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LARGE EDDY SIMULATION OF FIRE ACCIDENT DURING FLAMMABLE LIQUIDS TRANSPORT IN AN URBAN AREA*

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Dušica J. Pešić, Milan Đ. Blagojević, Nenad V. Živković, Ljiljana Đ. Živković, Miomir T. Raos

University of Niš, Faculty of Occupational Safety, Serbia

Abstract. *Air quality in urban areas has attracted great attention due to increasing pollutant emissions and their negative effects on human health and the environment. The aim of this paper is to analyze the impact of wind on air pollution and human vulnerability by fire products in an urban street canyon caused by a fire accident. For the simulation of a fire on a diesel oil truck a CFD Large Eddy Simulation method was used. Simulation results show that the fire product stream flows vertically upward, without touching the walls of the surrounding buildings in absence of wind. However, when the wind velocity reaches 6 m/s, the product stream curves towards the buildings at both sides of the street canyon. Concentrations of carbon monoxide and soot decrease, while carbon dioxide concentration increases with height. The described scenarios may lead to very serious situations, since circulating fire pollutants can be harmful for the people on the street as well as for those in the buildings with openings oriented toward the street canyon*

Key words: *flammable liquid, fire accident, products, air pollution*

1. Introduction

The problem of hazardous material transportation through heavily populated areas has received more attention during the last decades due to a significant increase in the public awareness of the potential dangers caused by chemical accidents and their effects on both inhabitants and the environment of urban settlements. Transport of oil and petroleum through urban areas occurs regularly because it is often nearly impossible to find alternative supply routes. For example, in our country, the transportation of flammable liquids accounted for an estimated 80% of the total quantity of hazardous material transportation, using all modes of transport within the area of Belgrade [4]. This transportation is hazardous because there is the possibility of leakage on road and, under certain circumstances, explosion and/or fire accidents may arise [2].

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Fire is followed by heat release, as well as by the formation of combustion products. The results of fires are products of incomplete combustion: carbon monoxide, nitrogen oxides, hydrogen cyanide and etc. Products of incomplete combustion and soot, as well as carbon dioxide as a product of complete combustion pollute the air and can affect climate change and have other effects on the environment. These pollutants can also lead to adverse impacts on the inhabitant's health. Accident prevention strategies call for thorough analyses of even worse scenarios when gaseous pollutants, as a result of a fire accident, might cause air pollution and an immediate threat for the exposed population [6].

In this paper, wind-driven dispersion of fire pollutants in a street canyon is analyzed. 'Street canyon' is a term frequently used for urban streets flanked by buildings on both sides and no major openings on the walls. The dimensions of a street canyon are usually expressed by their aspect ratio (the ratio of the street width W to the building height H) [1]. The wind flow pattern inside street canyons depends on their geometry, especially on the aspect ratio. The strength of the wind vortices inside the street canyon mainly depends on wind velocity at roof-top level. The Large Eddy Simulation (LES) method was used for the prediction of dispersion and concentrations of the fire pollutants in the street canyon.

2. NUMERICAL SIMULATION

2.1. The method

With the rapid development of computer technology, Computational Fluid Dynamics (CFD) modelling is nowadays widely applied for studies of turbulent flows (such as fire) and pollutant dispersion in an urban street. The turbulence methods commonly used in CFD include the Reynolds Averaged Navier-Stokes equation (RANS) method, Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS). The LES method has been recently widely used to simulate turbulent pollutant transport in fire-induced flow.

The Fire Dynamics Simulator (FDS), developed by National Institute of Standards and Technology (NIST), is now a popular CFD tool in fire-related studies, and suitable for the simulation of the concentration and flow distribution of fire products in an urban street. It solves numerically a form of the Navier-Stokes equations for thermally driven flow. The FDS is a CFD fire model used to compute gas density, velocity, temperature, pressure and species concentrations in each control volume. It solves the basic equations for a thermally expandable, multi-component mixture of ideal gases, as follows [5]:
Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = \dot{m}_b''' \quad (1)$$

Conservation of individual gaseous species:

$$\frac{\partial}{\partial t}(\rho Y_\alpha) + \nabla \cdot \rho Y_\alpha \mathbf{u} = \nabla \cdot \rho D_\alpha \nabla Y_\alpha + \dot{m}_\alpha''' + \dot{m}_{b,\alpha}''' \quad (2)$$

Conservation of momentum:

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot \rho \mathbf{u}\mathbf{u} + \nabla p = \rho \mathbf{g} + \mathbf{f}_b + \nabla \cdot \tau_{ij} \quad (3)$$

Transport of sensible enthalpy:

$$\frac{\partial}{\partial t}(\rho h_s) + \nabla \cdot \rho h_s \mathbf{u} = \frac{Dp}{Dt} + \dot{q}''' - \dot{q}_b''' - \nabla \cdot \dot{q}'' + \varepsilon \tag{4}$$

where ρ – density; **u** – three components of velocity, $\mathbf{u} = [u,v,w]^T$; T – temperature; D_α – diffusion coefficient; Y_α – mass fraction of αth species; $\dot{m}'''_{b,\alpha}$ - production of species α by evaporating particles; p – pressure; **g** – acceleration of gravity; $\mathbf{f}_b$ – external force vector; τ_{ij} – stress tensor; h_s – sensible enthalpy; $\dot{q}'''$ – heat release rate per unit volume from a chemical reaction; $\dot{q}_b'''$ – energy transferred to the evaporating droplets; $\dot{q}''$ – conductive and radiative heat fluxes; ε - dissipation rate and t - time.

The combustion model is based on the mixture fraction concept, which is quantitatively represented by the fuel and products of combustion. The reaction of fuel and oxygen is described as follows:

$$C_xH_yO_zN_aM_b + v_{O_2}O_2 \rightarrow v_{CO_2}CO_2 + v_{H_2O}H_2O + v_{CO}CO + v_S S + v_{N_2}N_2 + v_M M \tag{5}$$

Toxic pollutants (i.e. combustion products) that are formed under the studied process are:

$$v_{CO2} = x - v_{CO} - (1 - X_H)v_S \tag{6}$$

$$v_{CO} = \frac{W_F}{W_{CO}} y_{CO} \tag{7}$$

$$v_S = \frac{W_F}{W_S} y_S \tag{8}$$

$$W_S = X_H W_H + (1 - X_H)W_C \tag{9}$$

where v_k – the stoichiometric coefficient of species k; y_k – yield of species k; W_F – the molecular weight of fuel; W_k – the molecular weight of species k and X_H – the hydrogen atomic fraction.

The mixture fraction is defined in terms of the mass fractions of fuel (C_xH_y) and the carbon-carrying products of combustion:

$$Z = \frac{1}{Y_F^I}\left(Y_F + \frac{W_F}{xW_{CO2}} Y_{CO2} + \frac{W_F}{xW_{CO}} Y_{CO} + \frac{W_F}{xW_S} Y_S \right) \tag{10}$$

where Y_F^I – stands for the fuel mass fraction in fuel stream and Y_k – mass fractions of the species in the mixture.

2.2. Model configuration

FDS requires the following inputs: the geometry of the facility, computational cell size, location of the ignition source, fuel type, heat release rate, material thermal properties and boundary conditions.

A computational domain (22.5 m wide, 36 m long and 36 m high) was designed for CFD simulation. The building rows at two opposite sides of the domain are used to form a street canyon. Thus, a so called "regular" street canyon has been designed with an aspect ratio of one (the street width and the building height are set at 16 m). The buildings are assumedly made of concrete. The physical model for LES simulation is shown in Figure 1.

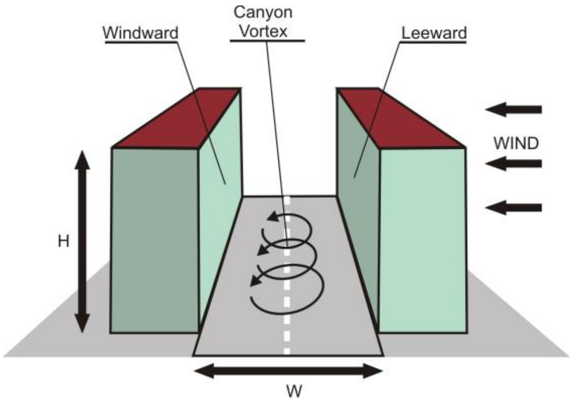

Fig. 1 The physical model for the LES simulation

When using the LES simulation, the grid size is a key parameter which has to be considered very carefully. For this investigation, the grid was uniform at 0.3 m in the three spatial directions (the *x*-, *y*- and *z*- direction). The number of grid cells was 1,080,000 (75×120×120 in the *x*, *y* and *z*- direction, respectively).

Accidental fires resulting from fuel spills and tank explosions commonly burn as pool fires. A large pool fire (i.e. diesel oil truck) was set as a buoyancy source at the center of the street canyon. A reaction type of "CRUDE OIL" according to the FDS reaction database [5] was specified for generating smoke and combustion products from the fire source. The buoyancy release rate of a fire is generally quantified by its Heat Release Rate per Unit Area (HRRPUA). A burning car or bus typically produces a fire with a heat release rate of 5 MW and 20 MW, respectively [3]. Since the tanker carries 15,000 l of diesel oil, the corresponding heat release rate of the burning truck is 230 MW. The HRRPUA for fire source was considered to be 4,500 KW/m^2. The conditions of "real" fire have been defined by parameters `SURF_ID='FIRE'` and `RAMP_Q='fireramp'` in the input file.

For the model of atmospheric air flow, the instantaneous or "real" wind has to be specified. An initial velocity boundary condition of 0.3 m/s was set at the right side of the simulation domain. The top and the other three sides of the domain were all set to be naturally open.

The simulations were carried out for different conditions: in the first case, the impact of wind on the dispersion of fire products was not taken into consideration while in the second, the impact of different values of wind velocity (2 m/s; 4 m/s; 5 m/s; 6 m/s and 8 m/s) were taken into consideration.

3. RESULTS AND DISCUSSION

Smoke movement is one of the basic and most important parts of a fire risk analysis. Therefore, the described simulations of a fire accident were meant to uncover the dispersion and concentrations of pollutants in the street canyon.

3.1. Dispersions of fire pollutants

The dispersions of fire pollutants under the influence of different wind velocities are shown in Figure 2.

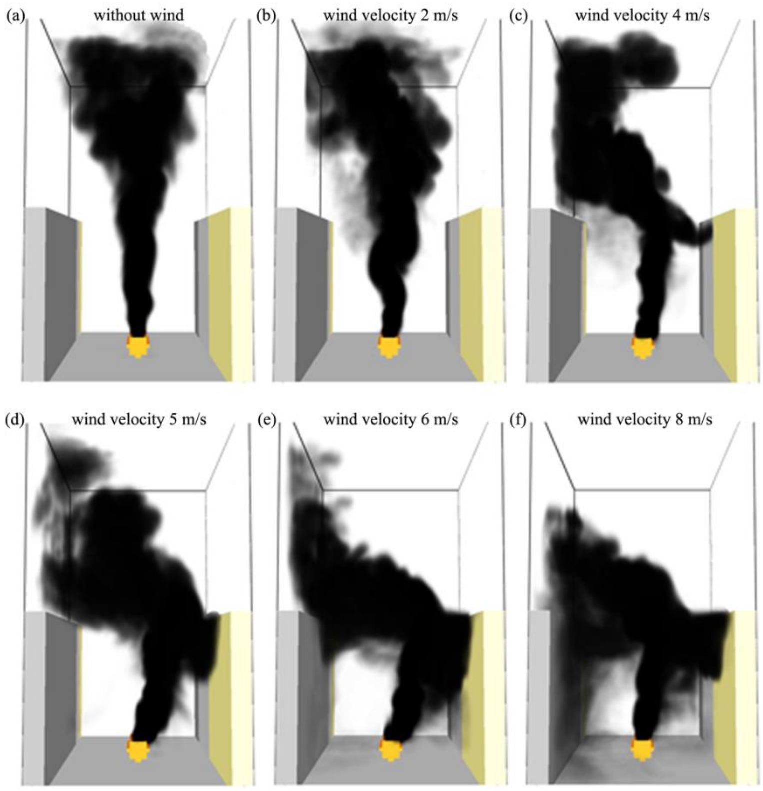

Fig. 2 The stream of fire products under different wind velocities

The results of fire product dispersion simulations, obtained for different wind velocities depict three flow regimes, as follows:

- Regime I, without wind (i.e. velocity < 0.5 m/s) or with low wind velocities (i.e. 2.0 m/s). Without wind, fire products rise up straight vertically with a velocity of 10 m/s, entraining fresh air from the surroundings, and the radius of the fire product stream increases axis-symmetrically (Figure 2(a)). Under low wind velocity, the stream of products is faster than the wind. It does not touch the walls of the buildings on both sides of the street canyon (Figure 2(b)). All the fire products were ventilated out of the top of the street freely by the aid of its own buoyancy.

- Regime II, with moderate wind velocity (i.e. 4 m/s and 5 m/s). In this regime, a portion of the fire products accumulated in the leeward side of the street canyon and touched the windward building (Figures 2(c), (d)). The accumulated products will be dangerous for the people in the compartments in the top part of the windward building if there are openings to the street. However, the stream of fire products did not touch the wall of the building at the windward side of the street.
- Regime III, with strong wind velocities (i.e. 6 m/s and 8 m/s). In the fire growth stage, fire products intensively mix with surrounding air and the product stream significantly bends toward the wind direction. Then, the stream of products bends toward the buildings located on the leeward side of the street canyon. Later on, in the developed stage of the fire, the wind forces the product stream to change direction toward the buildings on the windward side of the street canyon. Attention should be drawn to the fact that a portion of the fire products is being re-entrained back into the street, along the walls of the buildings (Figure 2(e)). With the increase of wind velocity, almost all the products were re-entrained back into the street. The products mostly accumulate in the streets with poor natural ventilation due to its own buoyancy (Figure 2(f)). This is a serious situation as re-entrained fire products could be harmful and toxic both for the people in the street and for the occupants of the buildings with openings toward the street.

3.2. Fire pollutant concentrations

Concentrations of carbon monoxide, carbon dioxide and soot particles in the center of the product stream at different heights above the street canyon level (3 m, 8 m, 13 m and 18 m, respectively) for two scenarios (without wind and with wind velocity of 6 m/s) are shown in Figures 3-5.

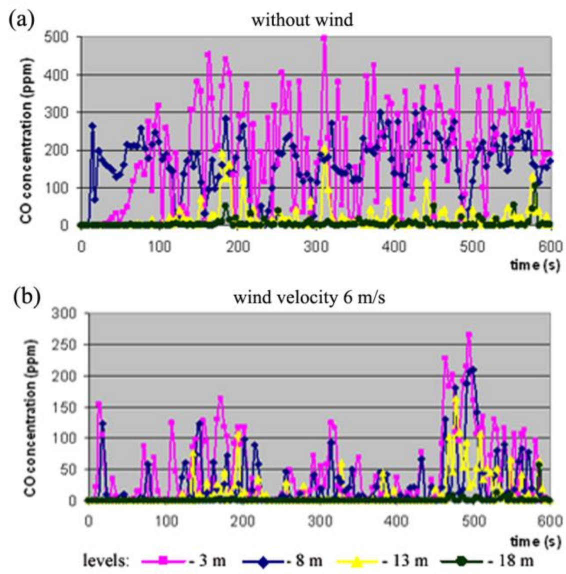

Fig. 3 Carbon monoxide concentrations

Carbon monoxide concentrations decrease with increasing height (Figure 3). This is explained by a two-step reaction of carbon. Namely, FDS comprises a methodology capable of taking into account incomplete combustion in the case of a large scale fire. The simplest possible two-step carbon monoxide formation mechanism is:

Step 1: $\mathrm{Fuel} + O_2 \rightarrow \mathrm{CO} + \mathrm{Other\ Products\ (i.e\ H_2O, soot)}$

Step 2: $\mathrm{CO} + \frac{1}{2} O_2 \rightarrow CO_2$

Carbon monoxide is an intermediate product obtained during flaming combustion. In the following step, carbon dioxide is generated as a product of complete oxidation.

Carbon monoxide concentration is correlated with air velocity and intensity of turbulence. The reason for higher concentrations of carbon monoxide in scenario without wind is the lack of oxygen necessary for achieving complete combustion (Figure 3(a)).

Figure 4 shows the fluctuation of carbon dioxide concentrations in time, measured at four different levels above the street canyon ground level.

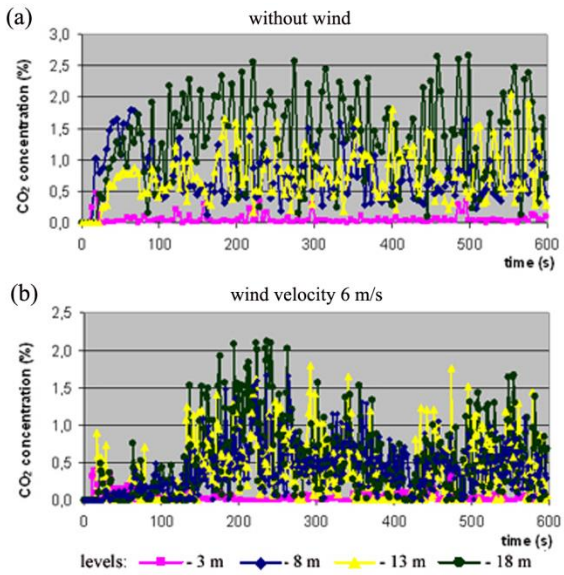

Fig. 4 Carbon dioxide concentrations

The more distant from the fire source, the higher the local carbon dioxide concentrations in the pollutant stream. Namely, carbon dioxide concentrations increase with height. This is explained by a two-step reaction of carbon which, when heated to high temperatures, unites with oxygen and forms carbon monoxide first and then carbon dioxide. Analyses of carbon dioxide concentrations reveal fluctuating behavior of carbon dioxide with time. Under exposure to wind, due to constant air inflow, combustion is more complete, so carbon dioxide concentrations increase (Figure 4(b)).

In effect of wind, complete combustion of fuel takes place due to a greater diffusion of oxygen to the fire center which result in the lower yield of combustion products containing carbon (equation (10)).

Soot particle formation during the fire is sign of oxygen deficiency. They are transported and distributed along with other combustion products, in the stream of fire pollutants. Soot has the longest life span as aerosol, and therefore, concentrations of it are of particular interest for air pollution investigation (Figure 5).

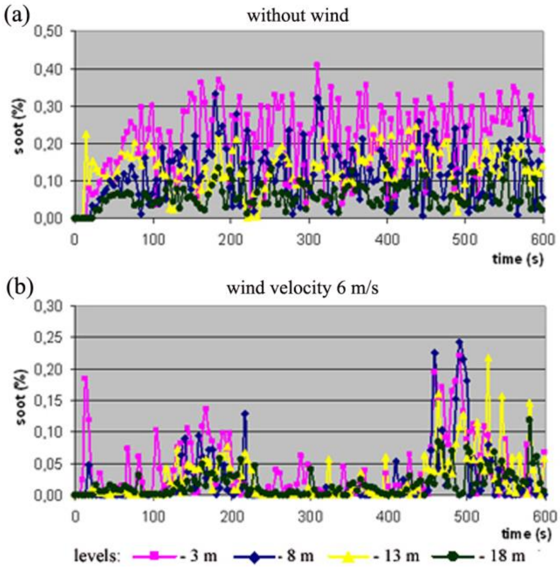

Fig. 5 Soot particles concentrations

The results of the simulations show that soot yield increases in under-ventilated fires. In the absence of wind, soot concentration over certain time instances exceeds the value of 0.4 % (Figure 5(a)). On the other hand, ventilation accelerates the combustion process, and the wind reduces soot concentrations from 0.2 % to 0.05 % (the described change in the concentration occurs in the time frame between 20 s and 450 s in the performed simulation). After that, soot concentrations increase again (Figure 5(b)).

3.3. Leeward and windward concentrations of pollutants

Wind causes the dispersion of fire pollutants toward the surrounding buildings contaminating air both on the lee and windward sides of the street canyon. Fields of carbon monoxide and carbon dioxide on the leeward and the windward side are shown in Figures 6-7.

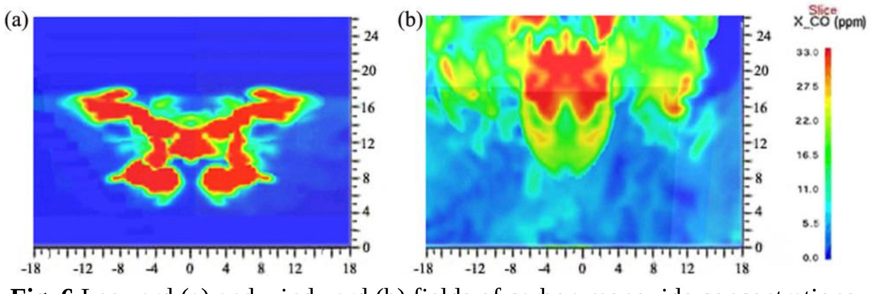

Fig. 6 Leeward (a) and windward (b) fields of carbon monoxide concentrations

At the times when fire product streams, driven by their own buoyancy, encounter the wind on the top of the street, they mix with the surrounding air. The increased leeward concentrations of fire pollutants are due to the accumulation of pollutants locally adverted by the large wind vortex that covers most of the street canyon.

Carbon monoxide affects the street level and the buildings on the leeward side of the street starting from 60 s in the simulation. High concentrations of carbon monoxide on the leeward side accumulate in a time interval of 230-450 s. Carbon monoxide, together with other products, returns from the roofs along the walls of the buildings on the windward side, all the way down to the street level.

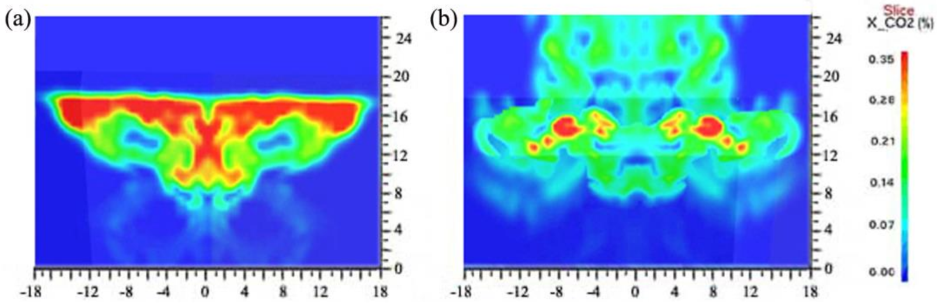

Fig. 7 Leeward (a) and windward (b) fields of carbon dioxide concentrations

Due to the two-step reaction of carbon with oxygen that ends up forming carbon dioxide at the higher levels, only upper floors of buildings on the leeward side of the street are jeopardized. However, during entire simulation, as a consequence of constant turbulence, carbon dioxide jeopardizes buildings on the windward side of the street canyon.

4. Conclusions

In this paper, the Large Eddy Simulation by Fire Dynamics Simulator was used to study the dispersion of fire-induced buoyancy-driven stream of fire products and fire pollutant concentrations in and above an urban street canyon.

The main purpose of this research was to explore impact of wind on the movement and concentrations of fire pollutants. Without wind or with low wind velocities, the stream of fire products did not touch the walls of the buildings on both sides of the street canyon. With moderate or strong wind velocity, the product stream curves to the walls of buildings. A portion of the fire pollutants were re-entrained back along the walls of the buildings, and reached the street level.

Predictions of distribution and concentrations of carbon monoxide, carbon dioxide and soot under the given circumstances were provided. The obtained results show that carbon monoxide and soot concentrations decrease with height, whereas carbon dioxide concentrations increase with height.

The described re-entrainment phenomenon of fire pollutants is very likely to occur in case of a fire accident in such a street. The existence of high risk and unforeseeable consequences that may arise in the case of accidents with hazardous materials during their transportation requires of all the participants in the transportation process to assume great responsibility, to have good training in working with such materials, knowledge of legal regulations and procedures, with constant control and supervision.

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MATEMATIČKI MODEL ZA TURBULENCIJU U UPOTREBI PRI SIMULACIJI POŽARA TOKOM TRANSPORTA ZAPALJIVIH TEČNOSTI U URBANOJ SREDINI

Kvalitet vazduha u urbanim sredinama je privukao veliku pažnju javnosti zbog povećanja emisije zagađujućih materija i njihovih negativnih uticaja na zdravlje ljudi i životnu sredinu. Cilj ovog rada je analiza uticaja vetra na disperziju produkata požara i zagađenje vazduha, kao i ugroženost ljudi u urbanoj ulici „kanjonu". Metod velikih vrtloga je korišćen za simulaciju požara cisterne sa dizel gorivom. Dobijeni rezultati pokazuju da se, u odsustvu vetra struja produkata požara kreće naviše ne dodirujući zidove zgrada. Međutim, kada brzina vetra dostigne 6 m/s, struja produkata se povija prema zradama sa obe strane ulice. Koncentracije ugljen monoksida i čađi opadaju, dok koncentracije ugljen dioksida rastu sa visinom iznad nivoa ulice. Opisani scenariji mogu dovesti do ozbiljne situacije s obzirom na činjenicu da produkti požara mogu da ugroze ljude koji se nalaze u ulici, kao i one u stanovima zgrada sa otvorenim prozorima.

Ključne reči: *zapaljiva tečnost, požar, produkti, zagađenje vazduha*