EFFECTS OF FIRE ON AIR

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The article below, gives an introduction on main toxic gases and their mechanisms, then in the uses a FDS Fire simulation to obtain data about the amount of pollutants that are issued into the air, in case of an accident happens: a large amount of kerosene, in the shape of a spill, burst into flames, affecting the environment.

Keywords: industrial fire, toxic gases, pollution, effects of fire.

1. Introduction

If we look up in the dictionary, fire is an oxidation process that releases energy in varying intensities in the form of light (with wavelengths also outside the visual spectrum) and heat and often creates smoke. It is commonly used to describe either a fuel in a state of combustion (e.g., a campfire, or a lit fireplace or stove) or a violent, destructive and uncontrolled burning (e.g., in buildings or a wildfire). Normally, the fire will have a general effect of heating the air, but also consumes oxygen, and issues smoke, soot and hot toxic gases, etc. Fires that affects environment in a greater percentage, are wildland (forest) and big industrial fires. This is why last part of the article presents a practical CFD method to predict the generation of toxic gases in open fires. The model makes use of local combustion conditions to determine the yield of carbon monoxide, carbon dioxide, soot and oxygen.

Fig.1.Greek forest fires. Satellite view

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Also, as an example of fire influence on the environment, should be reminded the series of forest fires burnt in Greece, especially in the Peloponnesus, with 68 confirmed casualties. Since June to August 2007, over 3 000 forest fires have raged the country (figure 1).

2. Normal atmosphere concentrations

The atmospheric air of the Earth is a mixture of gases with the main components being: nitrogen, oxygen, argon and carbon dioxide. It further contains traces of the other inert gases helium, neon, krypton and xenon.(see table I).

Table 1

Atmosphere concentrations

Mean composition of dry air in the troposphere	volume content in %	ppm (parts per million)
nitrogen (N)	78,08	780 800
oxygen (O_2)	20,95	209 500
argon	0,934	9340
neon	0,0018	18
helium	0,0005	5
krypton	0,0001	1
xenon	0,000009	0,09
carbon dioxide	0,035	350
methane	0,00017	1,7
dinitrogen monoxid	0,00003	0,3
carbon monoxide*	0,00002	0,2
hydrogen	0,00005	0,5

* carbon monoxide shows periodic changes

The atmosphere contains up to 4 % of water in all states of aggregation (contributes in certain conditions, to acid rains forming).

Up to 80 % of all water in the atmosphere is found in heights up to 3000 m. In the stratosphere, only 1 - 10 ppb (parts per billion) water is found.

Despite these relatively small amounts, water plays an important role in the atmosphere.

By phase transformations between gaseous, liquid and solid it is involved in energy transformation and transport and weather formation.

Because of its ability to absorb infrared radiation it plays an important role for the warming of the atmosphere.

3. Main Pollutants issued by fires. Acid rain forming

Carbon monoxide (CO), a toxic gas which is emitted into the atmosphere as a result of combustion processes, though thought of as a pollutant today, has always been present in the atmosphere. Carbon monoxide is created when carbon-containing fuels are burned incompletely. Through natural processes in the atmosphere, it is eventually oxidized to carbon dioxide. Carbon monoxide concentrations are both short-lived in the atmosphere and spatially variable.

Anthropogenic CO from automobile and industrial emissions may contribute to the greenhouse effect and global warming. In urban areas carbon monoxide, along with aldehydes, reacts photochemical to produce peroxy radicals. Peroxy radicals react with nitrogen oxide to increase the ratio of NO_2 to NO, which reduces the quantity of NO that is available to react with ozone.[5]

Carbon dioxide is a chemical compound composed of two oxygen atoms covalently bonded to a single carbon atom. It is a gas at standard temperature and pressure and exists in Earth's atmosphere as a gas. It is currently at a globally averaged concentration of approximately 385 ppm by volume in the Earth's atmosphere, although this varies both by location and time. Carbon dioxide's chemical formula is CO_2. In general, it is exhaled by animals and utilized by plants during photosynthesis. Additional carbon dioxide is created by the combustion of fossil fuels or vegetable matter, among other chemical processes.

Carbon dioxide is an important greenhouse gas because of its ability to absorb many infrared wavelengths of the Sun's light, and because of the length of time it stays in the Earth's atmosphere. Due to this, and the role it plays in the respiration of plants, it is a major component of the carbon cycle.

Soot and other airborne particulate matter vary widely in its physical and chemical composition, source and particle size. PM10 particles (the fraction of particulates in air of very small size (<10 µm)) are of major current concern, as they are small enough to penetrate deep into the lungs and so potentially pose significant health risks. Larger particles meanwhile, are not readily inhaled, and are removed relatively efficiently from the air by sedimentation. Particles are often classed as either primary (those emitted directly into the atmosphere) or secondary (those formed or modified in the atmosphere from condensation and growth). Major sources of fine primary particles are combustion processes.

Sulphur dioxide is a corrosive acid gas which combines with water vapors in the atmosphere to produce acid rain. Both wet and dry deposition has been implicated in the damage and destruction of vegetation and in the degradation of soils, building materials and watercourses. SO_2 in ambient air is also associated with asthma and chronic bronchitis.

Of particular concern in the past was the combination of SO_2 and black smoke and particulate matter; current EC Directive Limit Values for SO_2 are defined in terms of accompanying black smoke levels, although these are likely to change.

Nitrogen oxides are formed during high temperature combustion processes from the oxidation of nitrogen in the air or fuel. The principal source of nitrogen oxides - nitric oxide (NO) and nitrogen dioxide (NO_2), collectively known as NOx - is road traffic, which is responsible for approximately half the emissions in Europe. NO and NO_2 concentrations are therefore greatest in urban areas where traffic is heaviest. Other important sources are power stations, heating plants and industrial processes an fires.

Both nitrogen and sulfur oxides are known to react with water in the atmosphere to form acids. These reactions are the source of polluted acid rain.[5]

The formation of acid solutions by SO_2 is explained as a two - step process. Assume that sulfur dioxide molecules first react with water molecules, forming molecules of sulfurous acid:

$$SO_2(gas) + H_2O(liquid) \rightarrow H_2SO_3(aq) \qquad (1)$$

Sulfurous acid molecules then react with water producing an equilibrium with H+ (aq) and hydrogen sulfite. Sulfurous acid is considered a weak acid as it only partially ionizes into H+ (aq):

$$H_2SO_3\ (aq) + H_2O\ (liquid) \rightarrow H+\ (aq) + HSO_3\text{-}(aq) \qquad (2)$$

Sulfur dioxide can also react with oxygen or ozone to form sulfur trioxide:

$$2SO_2\ (gas) + O_2\ (gas) \rightarrow 2SO_3\ (gas)$$
$$SO_2\ (gas) + O_3\ (gas) \rightarrow SO_3\ (gas) + O_2\ (gas) \qquad (3)$$

The sulfur trioxide then reacts with atmospheric moisture to form sulfuric acid:

$$SO_3\ (gas) + H_2O\ (liquid) \rightarrow H_2SO_4\ (aq) \qquad (4)$$

This sulfuric acid is a strong acid that ionizes 100% in atmospheric precipitation to produce H+ (aq) ions:

$$H_2SO_4\ (aq) \rightarrow H+\ (aq) + HSO_4\text{-}(aq) \qquad (5)$$

These H+ (aq) are responsible for the acidic effects of acid rain.

Direct scavenging of NO_2 by atmospheric water contributes little nitric acid (HNO_3) on account of the low solubility of NO_2 in water:

$$2NO_2\ (gas) + 2H_2O\ (liquid) \rightarrow HNO_2\ (aq) + HNO_3\ (aq) \quad (6)$$

Acid rain containing considerable amounts of nitric acid likely originated without water:

$$NO_2\ (gas) + O_3\ (gas) \rightarrow NO_3\ (gas) + O_2\ (gas) \quad (7)$$

The gaseous NO_3 then reacts with any reactive hydrogen donor (X) in the atmosphere:

$$NO_3\ (gas) + XH\ (gas) \rightarrow HNO_3\ (aq) \quad (8)$$

Nitric acid like sulfuric acid is strong an completely ionizes into aqueous hydrogen and nitrate ions:

$$HNO_3\ (aq) \rightarrow H+\ (aq) + NO_3\text{-}(aq) \quad (9)$$

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.[4]

Fig.2. Fire modeling, main view (smoke) at time 580 s

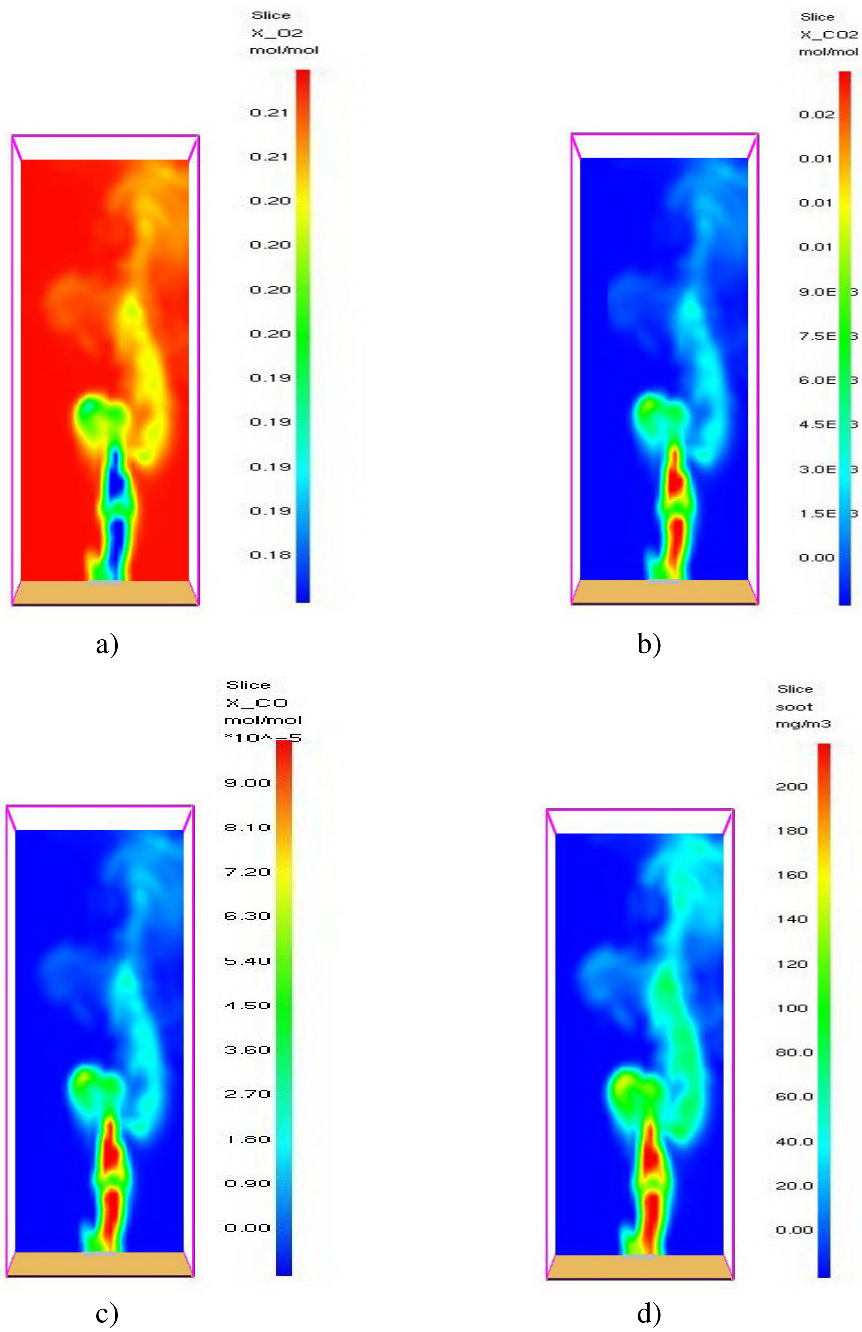

Fig.3. Fire simulation view of a) – oxygen, b) – CO, c) – CO_2, d) – soot of the kerosene spill, at time t 200 s

As a physical limitation of the mixture fraction approach to modeling combustion, we have the assumption that fuel and oxygen burn instantaneously when they are mixed. [1,2,4]

In the present research one have developed a three-dimensional model of a square shaped kerosene spill, which ignited, create the so called pool fire. The simulation is made in a computational domain with the dimensions: 30m width, 30 m length, and 80 m height. Total amount of cells involved in the hydrodynamic calculus is 144.000. The liquid fuel used for simulation is kerosene, with a spill thickness of 10 cm; the ambient temperature is 20° C, windspeed 0, 8 m/s and the total time duration for simulation is 600 seconds.

The simulations were conducted on a computer with 2400 MHz, Intel core 2 Duo processor and 1024 MB DDRAM.

Characteristics of the simulation: the spill diameter (the side of the square) is 6 m, wind speed is 0.8 m/s, and the program made 14425 reiterations in 8.27 hours.

5. Air Quality Standards

Humans can be adversely affected by exposure to air pollutants in ambient air. [3]

TableI1

Main atmosphere pollutants

Pollutant	Concentration	Averaging period	Permitted exceedences each year
Sulphur dioxide (SO2)	350 µg/m3	1 hour	24
	125 µg/m3	24 hours	3
Nitrogen dioxide (NO2)	200 µg/m3	1 hour	18
	40 µg/m3	1 year	n/a
PM10	50 µg/m3	24 hours	35
	40 µg/m3	1 year	n/a
Lead (Pb)	0.5 µg/m3	1 year	n/a
Carbon monoxide (CO)	10 mg/m3	Maximum daily 8 hour mean	n/a

In response, the European Union has developed an extensive body of legislation which establishes health based standards and objectives for a number of pollutants in air. These standards and objectives are summarized in the table II (extras).

6. Results and conclusions

In the simulation, at 200 s burning time results, as shown in picture 3, are as expected: Oxygen quantity drops rapidly near the flame, from 21% to a mere 1 %, CO_2 normally 0,035 %, raise up to 2 % - increase by 6 times, CO also raise from a normal limit of 0,2 ppm to 0,9 ppm, and soot raise from an accepted quantity of 50µg/m^3 to 200 mg/m^3. Improvements can be done to FDS program, to output also total volumes of toxic gases issued during every simulation.

Fires are important factors to take into consideration when assessing ways to control and minimize air pollution.

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