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## Effects of structural materials' chemical composition as considered in mathematical modeling built objects combustion processes

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# Effects of structural materials' chemical composition as considered in mathematical modeling built objects combustion processes

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**Abstract.** The article presents a symbolic (mathematical) model of combustion process alongside with its software implementation. The authors focus on effects of chemical composition of construction and finishing (decoration) materials involved in the process. The model was programmed before validation for adequacy and thus presents something more than description of chemical and physical moieties of combustion process.

## 1. Introduction

In fire condition it is lack of basic fire safety knowledge and skills that often results in people's deaths. More often than not it is not flame that causes death but pungent smoke and gas [1]. Any modern housing is accomplished with items and materials that can release over 70 various toxic substances when burnt. They are, abundantly, carbon monoxide, carbon dioxide, diphosgene, phosgene, hydrogen cyanide. And one could go on with the list. The longer you stay in a burning lodging, the less of a chance to survive you have. Statistics has it that over 50% of all those dying in fire condition die on the scene as a result of smoke inhalation. Casualties who manage to emerge get badly poisoned by pyretic chemicals and one in three dies in hospitals never regaining consciousness [2]. Smoke is an all-pervading attending circumstance in fire condition and it does cause death [3].

Fires entail casualties and aggravate the already unfavorable environmental conditions [4]. Combustion products that go to the atmosphere are in fact noxious emissions. As is known, industries and businesses are annually charged by the state for the negative effects to the environment, but it is disputable if the pay covers (in ecological terms) the real damage caused by such emergencies as accidental fires. Fire-related pollutant instances are difficult to calculate. That is why we regard as timely the objective of working out a symbolic (mathematical) model for evaluation of combustion-related emissions in fire condition.

It is not only a fire's physical characteristics such as speed of propagation and temperature that one needs to take into account while developing the model in question, but chemical composition of a premise's construction and decoration materials as well. The latter asks for splitting the model into two parts, a physical and a chemical one.

## 2. Selecting a method to calculate physical parameters of a fire event

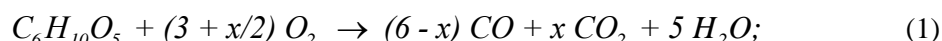
There are several methods for calculating spread of fire indoors. The zonal method appears to be the most commonly used in similar calculations. We find it appropriate for the present research study.



### 3. Analysis of combustion processes with structural and finishing materials

To analyze the combustion processes with structural and finishing materials, it is necessary to collect information on chemical composition of certain materials. Let us determine which materials we need to analyze. The common structural materials today are foam concrete, lime, gypsum sweep, portland cement, clays, cements, slag, steel, wood. However, when analyzing combustion processes, it is necessary to take into account not only structural materials, but finishing (decoration) materials as well. Here we evaluate the chemical composition of structural materials and their proneness to combustion. Most structural materials are either not prone to combustion at all, such as cement, glass, clay and brick, or glaze when heated, e.g. quartz sand. Consider combustion reactions in common combustible structural materials:

- wood, consists of cellulose  $C_6H_{10}O_5$ , combustion proceeds according to the reaction:

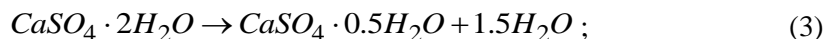


- steel, consists of iron and similar elements.  $Fe$  interacts with air oxygen  $O_2$  at the melting point of iron – 1538°C:



Other elements in the composition of steels also get oxidized to oxides, for example,  $CO$ ,  $CO_2$ ,  $P_2O_5$ ,  $NO_2$ ,  $SO_3$ ,  $SiO_2$ ,  $CrO_3$ ,  $Al_2O_3$ ,  $CuO$ ;

- quartz sand  $SiO_2$  – silicon oxide, does not burn, undergoes no chemical reactions, proves able to form glass;
- plaster, consists of gypsum, lime and cement:  $\alpha$ - gypsum  $CaSO_4 \cdot 2H_2O$  when heated to 150-180 °C passes into  $\beta$ -gypsum  $CaSO_4 \cdot 0.5H_2O$ :



- the hydrated lime of  $Ca(OH)_2$  passes into a non-quenched  $CaO$ :



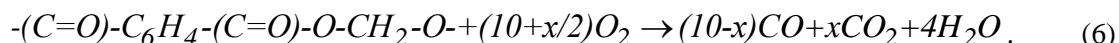
To render structuring of finishing materials more convenient, let us consider separately the materials that constitute the floor, ceiling, walls, windows, details of the interior and entrance doors.

Here we begin by writing out the equations of combustion reactions in finishing materials.

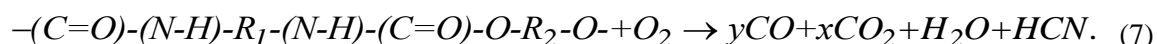
Polyvinyl chloride ( $-CH_2-CHCl-$ )<sub>n</sub> is part of many materials. At temperatures above 110-120 °C it is prone to decomposition with the liberation of hydrogen chloride  $HCl$ . At high temperatures, combustion proceeds according to the reaction:



Polyester – ( $-(C=O)-C_6H_4-(C=O)-O-CH_2-CH_2-O-$ )<sub>n</sub> at temperature over 850°C clean-burns to  $CO$  and  $CO_2$ :



Polyurethane – ( $-(C=O)-C_6H_4-(C=O)-O-CH_2-CH_2-O-$ )<sub>n</sub> at temperatures over 850 °C clean-burns to  $CO$  and  $CO_2$ :



Similarly, we write out reaction for all finishing materials. Analysis of combustion reactions in finishing materials allows us to identify the main products: carbon monoxide, carbon dioxide, hydrogen chloride, hydrogen cyanide, styrene, ethylene benzene, toluene, benzene. Here we determine

their most dangerous concentrations. *CO* (carbon monoxide) – a lethal concentration of 0.4% within 20-30 minutes. *CO<sub>2</sub>* – a concentration of more than 30% in the air – instant loss of consciousness and death. *HCl* (hydrogen chloride) – a concentration of 75-150 mg/m<sup>3</sup> – is intolerable. *HCN* (hydrogen cyanide) – 120-300 mg/m<sup>3</sup> 30-60 minutes – life-threatening toxic phenomena, 240-360 mg/m<sup>3</sup> 5 minutes – death, 420-500 mg/m<sup>3</sup> – death. Styrene – 1.5 mg/m<sup>3</sup> – death (tested on rats). Ethylene benzene – 1 mg/m<sup>3</sup> – malfunctioning of liver, 10 mg/m<sup>3</sup> – inflammation of the mucous membrane of the respiratory tract, 100-1000 mg/m<sup>3</sup> – cause functional and organic changes. Toluene – 250-500 mg/m<sup>3</sup> – death. Benzene – more than 3200 mg/m<sup>3</sup> – neurotoxic symptoms.

#### 4. Developing a mathematical model

The initial data for the related physicochemical problem are: the geometric dimensions of the room, materials of interior decoration and walls, location of windows and doors as fresh air flow agents. Relying on the initial data and using the zonal method, it appears possible to calculate the necessary physical parameters of a projected fire.

According to the chosen method, the average volume temperature at time  $t$  will be:

$$T = 115.6 \cdot \left( \frac{t}{t_{max}} \right)^{4.75} \cdot e^{-4.75(t/t_{max})} \cdot (T_{max} - T_0) + T_0, \quad (8)$$

where  $T_0$  – is the initial temperature,  $T_{max}$  – is the maximum average volume temperature,  $t_{max}$  – is the time to reach the maximum temperature.

The maximum temperature for a fire, regulated by a load, is given by the formula:

$$T_{max} - T_0 = 224 \cdot q_k^{0.528}, \quad (9)$$

where  $q_k$  – is the fire load value.

If the fire is regulated by ventilation, then the maximum temperature will be equal to one thousand degrees Celsius.

Time to reach the maximum average volume of temperature in case of a fire event regulated by the load:

$$t_{max} = 32 - 8.1 q_k^{3.2} \cdot e^{-0.92 q_k}. \quad (10)$$

In case of a fire event, regulated by ventilation, the maximum fire event time  $t_{max}$  will be calculated by the formula:

$$t_{max} = \frac{\sum P_i Q_{H_i}^p}{6285 \cdot A \cdot \sqrt{h}} \cdot \frac{n_{cp} \sum P_i}{\sum n_i P_i}, \quad (11)$$

where  $P_i$  – is the total amount of the fire load of the  $i$ -th component,  $Q_{H_i}^p$  – is the net calorific value of the  $i$ -th element of the fire load,  $h$  – is the height of the room openings,  $n_{cp}$  – is the average burn-up rate of the wood,  $n_i$  – is the average burning rate of the  $i$ -th component.

To determine if the fire will be regulated by ventilation or load, it is necessary to calculate the value of the fire load and the critical value of the fire load.

$$q_k = \frac{\sum P_i \cdot Q_{H_i}^p}{(6S - A) \cdot Q_{H_0}^p}, \quad (12)$$

where  $S$  – is the floor area of the room,  $A$  – is the total area of the room openings.

$$q_{kp.p.} = \frac{4500 \cdot \Pi^3}{1 + 500 \cdot \Pi^3} + \frac{V^{0.333}}{6 \cdot V_0}, \quad (13)$$

where  $P$  – is room openings,  $V$  – is room volume,  $V_0$  – is the total volume of air needed for combustion of the entire fire load.

If the value of the fire load is less than the critical value of the fire load, there will be a fire in the room regulated by the fire load. Otherwise, the fire will be regulated by room ventilability.

For rooms with volume of less than ten cubic meters, openings are calculated by the formula:

$$\Pi = \frac{\sum A_i h_i^{0.5}}{V^{0.667}}, \quad (14)$$

where  $A_i$  – is the area of the  $i$ -th opening of the room,  $h_i$  – is the height of the  $i$ -th opening of the room.

For premises with volume of more than ten cubic meters, the formula of openings appears as:

$$\Pi = \frac{\sum A_i h_i^{0.5}}{S}. \quad (15)$$

The total air volume required for combustion of the entire fire load is calculated by the formula:

$$\Pi = \frac{\sum V_i P_i}{\sum P_i}. \quad (16)$$

If we calculate emissions of a fire that has already happened, it is necessary to know the maximum temperature of the fire, while the volume of burned-out space is already known. The speed of propagation, too, can be calculated on the basis of burned-out space volume data.

The maximum temperature of the fire, regulated by the load, we find by the formula:

$$T_{max} - T_0 = 224 \cdot q_k^{0.528}, \quad (17)$$

where  $q_k$  – is the fire load value.

If the fire is regulated by ventilation, then the maximum temperature (to the accuracy of 5%) is found by the formula:

$$T_{max} = 940 e^{4.7 \cdot 10^{-3} (q - 30)}. \quad (18)$$

The calculation will take into account the influx of fresh air that provides the source zone of ignition with oxygen sufficient to maintain the chemical reaction. The amount of oxygen needed to sustain the combustion process is twenty-one percent of the enclosed space's total volume. During the combustion reaction, oxygen will be actively consumed in the oxidation and thermal decomposition processes. The intensity of these processes affects the amount of toxic substances released by the materials. The more oxygen is available for the combustion process; the more reactions will occur.

On the basis of the information obtained on the temperature and the percentage of oxygen in the air, it will be possible to find out what substances begin to emerge from the finishing and structural materials and at what point in time during oxidation and burning out.

The system (19) combines the equations of physics describing propagation of fire under various conditions, as well as chemical reactions taking place in the source of ignition. Thus, the system makes it possible to calculate the amount of chemical compounds released.

### 5. Developing a program for calculation pollutant emissions in case of fire

Data on the size of the room, the onset of ignition location, the initial temperature, and the time of the fire should be entered to the main window of the program. Room openings and height of the openings are to be calculated by the user based on the room's plan. In the Material section, one should enter the amount of material found in the room.

$$\left\{ \begin{array}{l} T = 115.6 \cdot \left( \frac{t}{t_{max}} \right)^{4.75} \cdot e^{-4.75(t/t_{max})} \cdot (T_{max} - T_0) + T_0; \\ T_{max} - T_0 = 224 \cdot q_k^{0.528}; \\ t_{max} = 32 - 8.1 q_k^{3.2} \cdot e^{-0.92 q_k}; \\ t_{max} = \frac{\sum P_i Q_{H_i}^p}{6285 \cdot A \cdot \sqrt{h}} \cdot \frac{n_{cp} \sum P_i}{\sum n_i P_i}; \\ q_k = \frac{\sum P_i \cdot Q_{H_i}^p}{(6S - A) \cdot Q_{H_0}^p}; \\ q_{kp.p.} = \frac{4500 \cdot \Pi^3}{1 + 500 \cdot \Pi^3} + \frac{V^{0.333}}{6 \cdot V_0}; \\ \Pi = \frac{\sum A_i h^{0.5}}{V^{0.667}}; \\ \Pi = \frac{\sum A_i h^{0.5}}{S}; \\ \Pi = \frac{\sum V_i P_i}{\sum P_i}; \\ V = a \cdot b \cdot h; \\ V_{O_2} = 0.21 \cdot V; \\ -CH_2-CHCl- + (2 + x/2) O_2 \rightarrow (2-x) CO + x CO_2 + H_2O + HCl; \\ -CH-(C_6H_5)-CH_2- + (6 + x/2) O_2 \rightarrow (8-x) CO + x CO_2 + 4 H_2O; \\ -CH-(C_6H_5)-CH_2- \rightarrow C_6H_5-CH=CH_2; \\ -CH-(C_6H_5)-CH_2- + (1.5 + x/2) O_2 \rightarrow C_6H_6 + (2-x) CO + x CO_2 + H_2O; \\ -CH-(C_6H_5)-CH_2- + H_2O \rightarrow C_6H_5-CH_2-CH_3 + 0.5 O_2; \\ CH-(C_6H_5)-CH_2- + (0.5 + x/2) O_2 \rightarrow C_6H_5-CH_3 + (1-x) CO + x CO_2; \\ C_6H_{10}O_5 + (3 + x/2) O_2 \rightarrow (6-x) CO + x CO_2 + 5 H_2O. \end{array} \right. \quad (19)$$

In addition, the program allows calculating payments for emissions to the environment according to the source [1]. To do this, one should enter the ready data on the substances already (data on

maximum permissible emissions, limits or information on the amount of emissions) to the table on the right of the main window. On introducing all necessary data, the results of calculation of payments for each hazardous substance separately as well as the total amount of payments for environmental pollution in the event of fire are displayed as a table.

## 6. Testing the program

As the test example, there is a room 5 meters high (height is  $a = 5$  m), 30 meters long (length  $b = 30$  m) and 70 meters wide (width  $c = 70$  m). The area of the room openings is  $A = 250$  m<sup>2</sup>, and their height is  $h = 4$  m. The initial temperature is set to 30 °C. The duration of fire is  $t_p = 30$  min. We assume that there are 20 tons of wood, 40 tons of polyvinyl chloride and 20 tons of foam plastic in the room.

We will calculate the example using the proposed mathematical model. For a start, we define the physical parameters of the fire:

$$V = a \cdot b \cdot c = 5 \cdot 30 \cdot 70 = 10500 \text{ m}^3. \quad (20)$$

$$S = b \cdot c = 30 \cdot 70 = 2100 \text{ m}^2. \quad (21)$$

$$q = \frac{\sum P_i}{S} = \frac{20000 + 40000 + 20000}{2100} = 38.09 \text{ kg / m}. \quad (22)$$

$$\Pi = \frac{\sum A_i \cdot h_i^{0.5}}{S} = \frac{250 \cdot \sqrt{4}}{2100} = 0.24 \text{ m}^{0.5}. \quad (23)$$

$$V_0 = \frac{\sum V_{0i} \cdot P_i}{\sum P_i} = \frac{4.2 \cdot 20000 + 5.4 \cdot 40000 + 8.44 \cdot 20000}{20000 + 40000 + 20000} = \frac{468800}{80000} = 5.86 \text{ m}^3. \quad (24)$$

$$q_{kp} = \frac{4500 \cdot \Pi^3}{1 + 500 \Pi^3} + \frac{V^{0.333}}{6V_0} = \frac{4500 \cdot 0.24^3}{1 + 500 \cdot 0.24^3} + \frac{10500^{0.333}}{6 \cdot 5.86} = 8.48 \text{ kg / m}^3. \quad (25)$$

$$q_k = \frac{\sum P_i \cdot Q_{H_i}^p}{(6S - A) \cdot Q_{H_0}^p} = \frac{20000 \cdot 13.8 + 40000 \cdot 20 + 20000 \cdot 41.63}{(6 \cdot 10500^{0.667} - 250) \cdot 13.8} = \frac{1908600}{36375.72} \text{ kg / m}^2. \quad (26)$$

$$q_k = 52.469 \text{ kg / m}^2. \quad (27)$$

We choose a fire with adjustable ventilation as the test case. We keep it in mind while calculating temperature:

$$T_{\max} = 940e^{4.7 \cdot 10^{-3} (38.09 - 30)} = 940e^{0.038} = 976.429^\circ \text{K}, \quad (28)$$

$$T_{\max} = 976.429 - 273.15 = 703.279^\circ \text{C}. \quad (29)$$

To determine what materials get burnt, we compare the combustion temperatures of materials with the maximum temperature found.

We find the burnt mass by the product of absolute mass velocity for the time of the fire in seconds:

$$M = V^{abc} \cdot t_n = 9.79 \cdot 1800 = 17623.62 \text{ kg.} \quad (30)$$

Further, it is necessary to separate the masses of individual materials from the total burnt-out mass.

To calculate the mass of substances released from burnt materials, chemical equations are needed. Let us calculate for polyvinylchloride:

$$CO_2 = 1.4 \cdot 8811.81 = 12336.53 \text{ kg,} \quad (31)$$

$$HCl = 0.2 \cdot 8811.81 = 1762.362 \text{ kg.} \quad (32)$$

A similar calculation is carried out for the remaining materials.

$$HCl = 1762.362 \text{ kg} \approx 1.76 \text{ ton,} \quad (33)$$

$$CO_2 = 12336.53 + 3392.5468 + 7490.038 = 23219.115 \text{ kg} \approx 23.22 \text{ ton,} \quad (34)$$

$$CO = 4317.7869 + 4846.49 = 9164.2769 \text{ kg} \approx 9.16 \text{ ton.} \quad (35)$$

We unite the masses according to the types of substances and select among them only those the owner is obliged to pay for. Payment is calculated according to the technique specified in [1].

The result of the programmed calculations work coincides completely with manual calculations. Therefore, the proposed software proves applicable for the research-related calculations.

## References

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