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# Features of modeling the combustion processes of flammable liquids with high ignition temperature in FDS software

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Abstract. The article describes the features of modeling the dynamics of fire during the combustion of flammable liquids, linked with dependence of the velocity of spreading along the liquid surface from a large number of factors. The method of computer simulation of combustion processes of flammable liquids with high ignition temperature is viewed via the Fire Dynamics Simulator software on the example of turbine oil. The influence of the linear velocity of flame spreading over the surface of turbine oil on the dynamics of temperature changes of the gaseous medium in the room is explored. The results of dynamic modeling of turbine oil combustion for cases of a simultaneously ignited area of the spilled flammable liquid and spreading of the flame over its surface from the ignition point with a calculated linear speed. The conclusion is made that it is expedient to use the described method for estimating the linear velocity of flame movement over the liquid surface when modeling combustion over large areas of flammable liquids with a high ignition temperature.

# 1. Introduction

Mathematical modeling of the dynamics of fire hazards for various scenarios of its development using software is one of the most important stages of fire risk assessment at production facilities [1]. However, the solution of this problem with burning flammable liquids (FL) has a number of difficulties.

In general, the dynamics of liquid combustion depends on its characteristics (flash point, ignition temperature, heat of evaporation, etc.) and the initial temperature. Meanwhile the fire development depends largely on the nature of the fire in one case, or another: the burning liquid is gushing (with the release of combustible liquids with high pressure), spill fire (burning of liquid spilled on the floor), three-dimensional combustion of liquid spills on different levels (when leaking from a storage tank, not under the pressure, directed downwards). Hence, the linear speed of flame distribution along the surface of the liquid will depend not only on its fire-hazardous characteristics, but also on the speed of the spill.

On the other hand, the linear velocity of the flame front spreading depends on the temperature of the liquid. If the temperature of the liquid is not more than flash point, the flame movement speed is small. With an increase in the FL temperature, the speed increases and reaches values corresponding to the distribution of the flame through the steam-air mixture. Therefore, depending on the intensity of heat radiation from the flame zone to the unburned neighboring areas of the liquid, as well as the relative location of the fire source and the FL spill zones, different fire dynamics will be observed at different levels [2].

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This article describes the features of computer modeling of combustion processes of flammable liquids on example of turbine oil in Fire Dynamics Simulator (FDS) software, used for modeling of development of the fire in room based on computational hydrodynamic model of heat and mass transfer during burning. The choice of turbine oil is due to the fact that its burning differs in high burn-out rate and high specific heat release.

# 2. Methods

The source data for the description of combustion processes in FDS are the stoichiometric coefficients for the combustion reaction, the number of atoms of each element in the molecule of the material, the molar mass of the fuel, the heat yield of the reaction, referred to the weight of oxygen, the maximum specific power of combustion, which are set by the user when configuring simulation. In addition, should take into account: the smoke-generating capacity of fuel, lower combustion value, specific rate of burnout, the coefficient of combustion efficiency, the linear velocity of flame spreading. It is reasonable to use information about the properties of substances given in various reference books [3-4], also, in some cases, calculation methods for determining the fire and explosion hazard of substances and materials [5].

When modeling a fire using FDS, by default, the program assumes that the entire surface of the FL mirror is instantly covered with flame, i.e. the linear velocity of the flame spreading over the liquid surface from the ignition source is considered to be infinitely large. As noted above, this value is finite and has certain values depending on specific conditions.

In the FDS software environment, it is possible for the user to independently set the linear velocity of flame spreading along the liquid surface. In reference [3-4] and normative literature, there is often no information about this value for FL. The calculation method for determining the maximum flame spreading velocity over the liquid surface [5] is applicable for the case when the initial temperature of the FL significantly exceeds the lower temperature limit of its ignition. This condition does not correspond to the initial conditions of the simulation of the combustion turbine oil which has a temperature lower flammability limit of 148 °C [3], which is much higher than the initial temperature of the liquid, even with the possibility of heating during the working cycle. In [6], only the approximate value of the flame spreading speed over the spilled oil product is indicated, which is 0.05 m/s for a liquid with a temperature below the flash point. In [7] based on the results of a research of spreading speed of the flame above the flammable liquid spill, the formula for estimating of linear speed of flame movement for FL with a high temperature of flash is presented:

$$V_l = \frac{A}{T_{inf} - T_0} \tag{1}$$

where  $V_l$  is the linear speed of flame spreading, cm/s; A = 28 cm·°C/sec – coefficient (in practice, to ensure the supply is doubled);  $T_{inf}$ ,  $T_0$  – accordingly, the ignition temperature of the FL and its initial temperature, °C.

The limitations of this method should be taken into account. In particular, formula (1) does not consider the dynamics of liquid movement during spreading, as well as the increase in the speed of flame movement when the liquid is heated by radiation. It should be noted that for large areas of spillage, the linear velocity of flame spreading over the surface of the FL can have a significant impact on the development of a fire, especially at the initial stage.

These factors create complexity and uncertainty in the choice of the algorithm for simulation of combustion. Bearing in mind the changes in the parameters of the flammable liquid discussed above, modeling the development of a fire during its burning does not always give a reliable result.

## 3. Results

To assess the influence of the linear velocity of flame spreading over the FL surface on the fire dynamics, two computer experiments were performed in the FDS program (using the PyroSim graphical interface),

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where the main fire load is TP-22C turbine oil spilled on several levels (0 m, 4 m, 8 m, 12 m) with a total area of about 200 square meters (figure 1):

Experiment 1 - at the start of the simulation, the entire surface of the FL spill is ignited, i.e. the linear velocity is assumed to be infinitely large.

Experiment 2-the flame spreads along the surface of the liquid from the ignition source at a linear speed calculated by the formula (1).

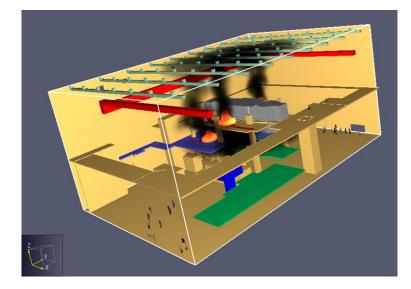
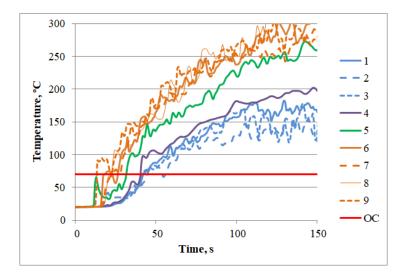


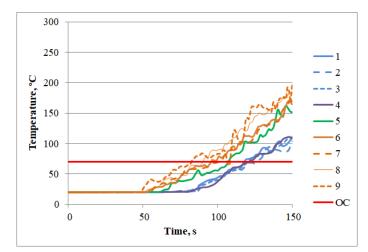
Figure 1. Computer experiment model.

This fire scenario is characterized by a significant total area of spilled oil, reaching several hundred square meters, according to the high volume of the turbine oil lubrication system. Consequently, the differences in the dynamics of fire development with the gradual spread of the flame along the surface of the FL mirror from the ignition source and with its instantaneous ignition are most noticeable. Figures 2 and 3 present time graphs of the temperature of the gas medium at various points in the room, obtained as a result of modeling in the FDS software environment, as well as the time when it reaches the overload capacity for a person (OC).



**Figure 2.** Time graphs of the temperature of the gas medium (experiment 1) on levels 0 m (points 1-3), 4 m (point 4), 8 m (point 5), 12 m (points 6-9).

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**Figure 3.** Time graphs of the temperature of the gas medium (experiment 2) on levels 0 m (points 1-3), 4 m (point 4), 8 m (point 5), 12 m (points 6-9).

## 4. Discussion

As follows from the results obtained, in the case of instantaneous ignition of FL (experiment 1), the temperature at the calculated points at various levels reaches the overload capacity during the first 10-45 seconds of the fire, amounting to 120-310 °C at the end of the simulation. With the gradual spread of the flame (experiment 2), the temperature values grow more slowly, the OC at various levels is exceeded after 80-125 seconds from the start of the fire, the maximum achieved values of the gas medium temperature are in the range of 100-200 °C.

Such a difference in the results obtained at the initial stage of a fire in some cases may be critical, in particular when studying the execution of the conditions for safe evacuation of people in a fire under the considered scenario, the probability of collapse of building structures, etc.

## 5. Conclusion

Thus, the choice of the speed of flame spreading over the surface of a flammable liquid can significantly affect the results of the study when evaluating the dynamics of a fire. This effect is especially significant at the initial stage of the fire. Therefore, when modeling combustion processes associated with a FL spill with a high ignition temperature, especially over large areas, it is advisable to use the recommendations presented in [7] to estimate the linear velocity of the flame movement over the liquid surface, the limitations of the method included.

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