Simulation of Liquid Fuel Spills Combustion Dynamics Based on Computational Fluid Dynamics Using Modern Application Programs

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Abstract. The article presents the results of calculations using modern application programs, using the CFD FDS 6.3 model, self-sustaining burning of liquid hydrocarbon fuel spills with a sufficiently high accuracy for spills less than 0.5m in diameter. The study shows that the use of modern software systems for CFD modeling, taking into account wind direction, humidity and other environmental parameters, significantly reduces the costs of risk assessment in emergency situations associated with the use of LNG in transport. Conducted research allows to increase reliability and reduce risks of liquefied natural gas usage in transport.

1. Introduction

One of the developed countries transition manifestations to a new technological level is the rapid development of power plants [1] and the growing use of alternative fuels, among which the most promising is natural gas.

In systems containing flammable liquids, there is always risk of accidental leakage. Inflammation of liquids can result in a fire that threatens people, structures, or the environment. Such fires occur rarely, however, when they occur, they require significant resources for successful extinguishing. Risks of fires over spills of liquid fuels are present at all stages of the processing and operation of systems associated with hydrocarbons [2].

When designing new fire extinguishing systems or upgrading existing ones, it is necessary to estimate the combustion parameters as accurately as possible. For this purpose, experimental studies and numerical modeling are used. The latter significantly reduces cost of development.

The quantitative prediction of the fuel burnout rate and heat release rate in flame is an important task of modeling fire dynamics. Modern methods of numerical simulation of combustion above the liquid surface are characterized by separate modeling of processes in the gas and liquid phases, within predetermined rate of fuel evaporation is used in gas-phase combustion calculations. [3, 4]. This approach requires the use of empirical data for the rate of the fuel burnout and does not take into account its possible changes (for example, under the influence of side wind [5]). Joint simulation of gas-phase combustion and evaporation of liquid fuel is a more complicated task, for which it is necessary to take into account the dependence of the liquid evaporation rate of the heat flow from the gas-phase flame (thermal feedback).
Thus, one of the most important and relevant scientific and technical problems of water transport is a study aimed at assessing the safety of the use of liquefied natural gas on ships.

2. Main part
It is known that LNG is a flammable cryogenic liquid and therefore represents a safety hazard. The extensive use of LNG in the maritime sector requires appropriate means of transportation, storage and bunkering. It is required to analyze the risks associated with the operation of these objects. Specific safety characteristics of the equipment involved should be included in the analysis and laid the foundation for modern ship systems projects [6, 7]. Safe distances should be determined on the basis of studying the consequences of accidents at facilities associated with LNG, at the moment there are a lot of requirements for the safe operation of gas-powered vessels [8].

The burning of liquid fuel spills has been the subject of intense researches for several decades. Classical measurements of burnout rates for tanks of various sizes were carried out by Blinov and Khudyakov in 1961. The results presented in this paper are explained by Hottel (1959) and Sibulkin (1973) by comparing different types of heat transfer from the flame to the spillsurface. Since that time, numerous experimental studies have been presented (Hamins et al., 1994; Jansens, 2001; Klassen, 1992; Koseki, 1996, 1999; Natsumi et al., 1998) reviewing different types of fuels and reservoir sizes.

Today, modeling complex processes, using modern tools for analyzing, processing and presenting information, is an integral component for the effective management of any system are in development [9, 10, 11, 12].

The underlying and most important phenomenon in the study of the liquid fuel spills burning is the thermal connection between the fuel and the flame. This relationship determines the gasification, and it, in turn, significantly affects heat generation and, consequently, heat fluxes. The development of CFD models requires detailed experimental data on the structure of this relationship. Such information was presented in the works of Hamins et al. in 1994, Classen (1992) and Koseki (1996). Typically, the data includes burnout rates, radiated and total heat flux distributions, soot mass fractions and some other parameters.

Attempts to combustion CFD modeling of tanks with liquid fuel were made in a variety of studies (Mel et al., 1996. [13]; McGrattan et al. 1998 [14]; Sinai and Owens, 1995 [15]; Wang and Julian, 1997 [16]). These studies provide encouraging results for burning of limited and unlimited liquid fuel tanks. Most of these studies use the burnout rate of fuel as a model parameter or use simplified empirical patterns, as presented by Jansens in 2001. [17].

The full CFD model of liquid fuels burning must predict the burnout rate as part of complete solution, therefore, it is required to simulate the relationship between the gas and liquid phases. The burnout rate changes as the flame develops during the transition period and reaches a quasi-steady burning mode. Therefore, the CFD model should also consider a transitional period. This was produced only relatively recently. One example of such a study is the work of Prasad and others in 1999. [18]. In this study, the laminar flow equations are used to predict the combustion of a tank with methanol of 1 cm in diameter. The radiation was calculated in an optically thin approximation, suitable only for fuels with low soot formation.

The development of fire dynamics numerical modeling has led to the creation of a variety of mathematical models and program codes, the main ones are listed in the Combustion Science & Engineering, Inc. database [19].

The model of heat transfer in a liquid is presented in work [20], which is added to the FDS calculation code. The dependence of the results on the mass transfer coefficient and the temperature of the liquid surface is considered, on the basis of which the dependence is presented, reflecting the increase in the gasification rate with increasing mass transfer coefficient at the same surface temperature. The stability of the obtained maximum burnout rates from the specified properties of the fuel was studied. In this article, modeling is performed only for tanks with a side of more than 1m.
There is no sufficiently reliable, experimentally tested method for the joint simulation of the gasification of liquid fuel and turbulent gas-phase combustion. This hinders the use of existing models, including FDS and others, to predict fires in engineering practice and further researches.

The FDS CFD model solves the Navier-Stokes equations numerically in the approximation of small Mach numbers, thermally movable flows with special attention to smoke and heat flows. The model is a system of partial differential equations, including the equation of mass, momentum and energy conservation and is solved on a three-dimensional regular grid. Heat radiation is calculated by the finite volume method on the same grid. To simulate the movement of smoke, sprinklers and spraying fuel, Lagrange particles are used. The main goal of FDS throughout its development was to solve applied fire safety tasks and at the same time provide a tool to study the fundamental processes in a fire.

To joint simulation of the liquid combustible material pyrolysis and the turbulent combustion of its gasification products, the experiments presented in the article are used as a scenario [21]. Heptane and ethanol were selected as the reference fuels based on the maximum heights of the non-smoking flame. The centers have the shape of a square and are in the center of the calculated area lower boundary, the thickness of the fluid layer is 0.05 m. The surface of the lesions is located at the same level with the lower surface of the calculated region. The bottom surface is impenetrable and maintained at a constant temperature of 25°C. The calculated area is a cube with a face equal to two heights of the flame, calculated according to the Heskstad formula [4] based on the flame height estimate of the specific heat generated in the experimental data [21, 22].

Fig. 1 shows the graphs of specific heat release rate for burning heptane in a 0.1m tank with grids: 20x20x20, 80x80x80, 160x160x160 cells.

Based on the results presented in Fig. 2 it can be argued that the initial ambient temperature does not have a significant effect on steady-state combustion, but if the initial ambient temperature is set to 77°C, it takes much less time to achieve a quasistationary combustion mode.

![Figure 1](image1.png)  
**Figure 1.** Dependence of specific heat release on time for a 0.1 m tank for three grids.

![Figure 2](image2.png)  
**Figure 2.** The dependence of specific heat generation on time when burning a ethanol tank with a side of D = 1 m.

When performing calculations on the 160x160x160 grid, the heat generation averaged over the steady-state combustion area is 30% less than when using the 80x80x80 grid, further refinement of the grid design resulted in a slight change in the average heat generation, with an increase in the required time for more than 3 times Therefore was used grid of 160x160x160 cells.

Fig. 3 shows the dependence of heat generation rate for heptane, and for ethanol on Fig. 4. can be seen that with large tank diameters the heat release rate is greatly underestimated.
The type of flame for different sizes of the spill (the isosurface of the heat release rate of 200 kW/m²), as well as the instantaneous temperature fields in axial section, are shown in Fig.5.

**Figure 3.** Heat release rate for fuel: Heptane \((C_7H_{16})\)

\[ \Delta H_g = 493 \text{ kJ/kg} \quad \Delta H_c = 4.356 \cdot 10^4 \text{ kJ/kg} \]

**Figure 4.** Heat release rate for fuel: Ethanol \((C_2H_5OH)\)

\[ \Delta H_g = 880 \text{ kJ/kg} \quad \Delta H_g = 2.7 \cdot 10^4 \text{ kJ/kg} \]
According to the obtained dependence of specific heat release rate on the size of the spill, the following conclusions can be drawn: the heat emission obtained as a result of these calculations correlates with the experimentally measured for tanks from 0.1 to 0.3 m in size, and for tanks from 0.5 to 1, the calculated heat release rate is much lower than the experimental one. In particular, for a 1m heptane reservoir, the discrepancy with the experimental data is about 30%.

Consider the dependence of the averaged heat flux on the liquid surface of the tank size. It can be seen that heat flux obtained by the liquid is much greater than the radiant heat flux incident on it, measured experimentally in the work [21], due to the fact that the convective component, that is not taken into account in an experimental study, plays a large role with small burners. Calculated heat flux best of all agrees with the data presented in the article [21] for a tank with a side D=1 m.

3. Conclusion
Thus, the review and classification of the available data on the burning of liquid fuels spills under flammability tests and real fire conditions allows us to conclude that the obtained analytical dependences for modeling using modern application programs, for example using the CFD FDS 6.3 model, are applicable to analysis and risk assessment of emergencies associated with spills of liquid fuels.

The performed numerical experiments on combustion of heptane and ethanol, taking into account the dependence of the fuel evaporation rate on the heat flux created by the flame, have shown that: the FDS model reproduces well the qualitative dependence of convective and radiant heat fluxes ratios obtained by the spill surface of liquid fuel, and the FDS 6.3 model and code can produce calculation of
self-sustaining combustion of spills of liquid hydrocarbon fuels with a sufficiently high accuracy for liquid fuels spills less than 0.5 m in diameter.

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