

Mathematical modeling of heat and mass transfer processes at the ignition of a liquid condensed substance by an immersed hot particle

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Abstract. A numerical investigation of heat and mass transfer processes at the heating of combustible liquid was carried out at the interaction of hot small-size steel particle with gasoline. Developed mathematical model considers at two-dimensional statement thermal conduction, thermal convection, transfer of energy by phase change (evaporation of liquid fuel and crystallization of particle material), partial immersion of hot particle in liquid fuel, forming of vapor gap between hot particle and liquid fuel, diffusion of fuel vapors in oxidizer, dependence of thermophysical characteristics of interactive substances on temperature. It was established that the highest rates of heat and mass transfer processes in a system “hot particle – gasoline – air” are possible at temperature of hot particle higher than melting temperature of it material due to the additional heat released at the crystallization of material.

1. Introduction

Heating, evaporation and ignition of liquid condensed substances drops at contact with hot plate are strongly investigated [1–6]. Such interest can be explained by absence of information about main regularities of interconnected heat and mass transfer processes. Heating, evaporation and ignition of liquid condensed substances by local energy sources with small sizes (for example, heated till high temperatures metallic and nonmetallic particles with limited heat content) is known less.

Interaction processes between heated particles formed at cutting, welding and friction of metals with solid and liquid combustible substances are significant processes from the point of industrial safety. These processes are characterized by high rates of chemical reactions, heat and mass transfer, small sizes and high temperatures of energy sources, consequently high fire density.

The general ignition theory for liquid combustible substances at different mechanisms of energy supply (thermal conduction, thermal convection, and thermal radiation) is not developed. However similar theory for solids combustible substances exists [7–9]. This result can be explained by more difficult heat and mass transfer mechanisms for liquids in comparison with solids, and absence of experimental data.

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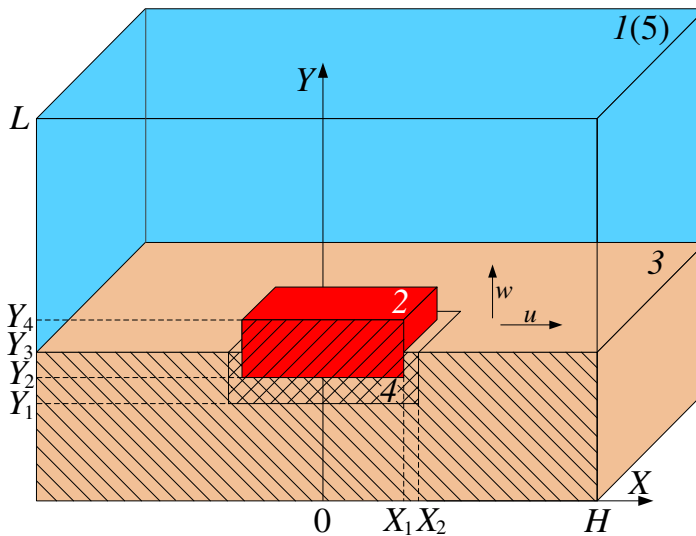


Figure 1. A scheme of the solution domain area: 1 – air (at $\tau = 0$), 2 – hot particle, 3 – liquid fuel, 4 – vapor gap, 5 – mixture of fuel vapors and air (at $0 < \tau \leq \tau_d$).

Nowadays results of theoretical investigations of ignition processes of typical liquid fuels by single heated till high temperatures steel particle are known [10–12]. A few factors influencing on heat transfer characteristics at the ignition were not considered at these papers. For example, the dependences of thermophysical characteristics on temperature for substances and possible processes transfer of energy by phase changes at the crystallization of hot particle material.

The purpose of present work is the numerical investigation of basis regularities for heat and mass transfer processes at immersion of a metallic hot particle in a liquid fuel. Mathematical model of process considers two-dimensional heat and mass transfer, kinetics of evaporation and ignition processes, crystallization of hot particle material, partial immersion of hot particle in liquid fuel, forming of vapor gap between hot particle and liquid fuel, and dependence of thermophysical characteristics of substances on temperature.

2. Problem statement

The problem of liquid fuel (gasoline) ignition by single hot steel particle was examined. It was supposed that local energy source (small sizes particle) fell into gasoline surface. Particle immersed in liquid (Fig. 1) and near-surface layer of condensed substance was heated. The evaporation began at the achievement of phase change conditions. The fuel vapor gap was formed between the energy source and the liquid fuel (Fig. 1). The rate of vapor gap was defined by the particle heat content, thermophysical and kinetic characteristics of liquid condensed substance. Fuel vapor got up and diffused at air. As the result flammable gas-vapor mixture was formed nearby contact boundary between the particle and the liquid. Ignition conditions for mixture realized at critical values of fuel concentration and its temperature.

Theoretical investigations of interconnected heat and mass transfer process in the system (Fig. 1) were carried out for parallelepiped-shape particle with sizes L_p ($L_p = X_1$) and H_p ($H_p = Y_4 - Y_2$). Sizes of solution area L and H were changed greatly more than L_p and H_p .

Follow ignition conditions were assumed [7]:

1. Heat released due to chemical reaction of fuel vapors oxidation is more than heat transferred from a hot particle to liquid condensed substance and air.
2. Temperature of gas-vapor mixture exceeds the initial temperature of a particle.

3. Mathematical model

System of transient differential equations [13, 14] for concerned gas-phase ignition process (Fig. 1) includes thermal convection equation, Poisson's equation, thermal conduction equation, diffusion equation and balance equation for fuel vapors in the air; thermal conduction equations for hot particle and liquid fuel. At dimensionless variables ($0 < \tau \leq \tau_d$):

$0 < X < X_2/L, Y_1/L < Y < Y_2/L; X_1/L < X < X_2/L, Y_2/L < Y < Y_3/L; X_1/L < X < H/L, Y_3/L < Y < Y_4/L; 0 < X < H/L, Y_4/L < Y < 1$

$$\frac{1}{\text{Sh}} \frac{\partial \Omega}{\partial \tau} + U \frac{\partial \Omega}{\partial X} + V \frac{\partial \Omega}{\partial Y} = \frac{1}{\text{Re}} \left[\frac{\partial^2 \Omega}{\partial X^2} + \frac{\partial^2 \Omega}{\partial Y^2} \right] + \frac{\text{Gr}}{\text{Re}^2} \frac{\partial \Theta}{\partial X}, \quad (1)$$

$$\frac{\partial^2 \Psi}{\partial X^2} + \frac{\partial^2 \Psi}{\partial Y^2} = \Omega, \quad (2)$$

$$\frac{1}{\text{Sh}} \frac{\partial \Theta_5}{\partial \tau} + U \frac{\partial \Theta_5}{\partial X} + V \frac{\partial \Theta_5}{\partial Y} = \frac{1}{\text{Re Pr}} \left[\frac{\partial^2 \Theta_5}{\partial X^2} + \frac{\partial^2 \Theta_5}{\partial Y^2} \right] + \text{Sr}_2, \quad (3)$$

$$\frac{1}{\text{Sh}} \frac{\partial C_f}{\partial \tau} + U \frac{\partial C_f}{\partial X} + V \frac{\partial C_f}{\partial Y} = \frac{1}{\text{Re Sc}} \left[\frac{\partial^2 C_f}{\partial X^2} + \frac{\partial^2 C_f}{\partial Y^2} \right] - \text{Sr}_1, \quad (4)$$

$$C_f + C_o = 1; \quad (5)$$

$0 < X < X_1/L, Y_2/L < Y < Y_4/L$

$$\frac{1}{\text{Fo}_2} \frac{\partial \Theta_2}{\partial \tau} = \frac{\partial^2 \Theta_2}{\partial X^2} + \frac{\partial^2 \Theta_2}{\partial Y^2} + \text{Sr}_3; \quad (6)$$

$0 < X < H/L, 0 < Y < Y_1/L; X_2/L < X < H/L, Y_1/L < Y < Y_3/L$

$$\frac{1}{\text{Fo}_3} \frac{\partial \Theta_3}{\partial \tau} = \frac{\partial^2 \Theta_3}{\partial X^2} + \frac{\partial^2 \Theta_3}{\partial Y^2}. \quad (7)$$

$\text{Sr}_1, \text{Sr}_2, \text{Sr}_3$ are dimensionless complexes ($\text{Sr}_1 = (HW_0)/(\rho_5(T)V_m)$, $\text{Sr}_2 = \text{Sr}_1 Q_o/(C_5(T)\Delta T)$, $\text{Sr}_3 = (Q_{cr}W_{cr}H)/(L_p\Delta T\lambda_2(T))$); t is time, s; t_d is ignition delay time, s; t_m is time scale, s; X and Y are dimensionless coordinates of Cartesian display correspond to x and y ; Sh is Strouhal number; Ω is dimensionless vortex velocity vector; τ is dimensionless time; τ_d is dimensionless ignition delay time ($\tau_d = t_d/t_m$); U and V are dimensionless rates of fuel vapors at projection on x and y ; Re is Reynolds number; Gr is Grashof number; Θ is dimensionless temperature; Ψ is dimensionless stream function; Pr is Prandtl number; Q_o is heat of oxidation reaction of fuel vapors in air, J/kg; W_o is mass rate of fuel vapors oxidation in air, kg/m³ s; ρ is density, kg/m³; C is specific heat, J/(kg · K); T is temperature, K; ΔT is differential temperature ($\Delta T = T_m - T_0$), K; T_m is temperature scale, K; T_p is initial particle temperature, K; T_0 is initial liquid and air temperature, K; V_m is rate scale of convection ($V_m = \sqrt{g\beta\Delta TL}$), m/s; g is gravitational acceleration, m/s²; β is solid coefficient of expansion, K⁻¹; C_f is mass concentration of fuel vapors in gas-vapor mixture; C_o is mass concentration of oxidant in gas-vapor mixture; Sc is Schmidt number; Fo is Fourier number; Q_{cr} is heat of energy source crystallization, J/kg; W_{cr} is mass rate of particle crystallization, kg/(m² · s); λ is thermal conductivity, W/(m.K); subscripts 1, 2, 3, 4, 5 correspond to air, hot particle, liquid fuel, fuel vapor, gas-vapor mixture.

Initial ($\tau = 0$) conditions:

$\Theta = \Theta_0, C_f = 0, \Omega = 0, \Psi = 0$ at $X_1/L < X < H/L, Y_1/L < Y < Y_2/L; 0 < X < H/L, Y_2/L < Y < 1$;

$\Theta = \Theta_p$ at $0 < X < X_1/L, Y_1/L < Y < Y_2/L$;

$\Theta = \Theta_0$ at $0 < X < H/L, 0 < Y < Y_1/L$.

Boundary ($0 < \tau \leq \tau_d$) conditions (Fig. 1):

on boundaries “particle – fuel vapor” ($Y = Y_2/L, 0 < X < X_1/L; X = X_1/L, Y_2/L < Y < Y_3/L$), “particle – gas-vapor mixture” ($Y = Y_4/L, 0 < X < X_1/L; X = X_1/L, Y_3/L < Y < Y_4/L$) boundary perfect thermal contact conditions were accepted for thermal conduction equations, besides condition of equality to zero gradients of corresponding functions for thermal convection, diffusion and Poisson equations were assumed;

on boundaries “liquid – fuel vapor” ($Y = Y_1/L, 0 < X < X_2/L; X = X_2/L, Y_1/L < Y < Y_3/L$), “liquid – gas-vapor mixture” ($Y = Y_1/L, 0 < X < X_2/L; X = X_2/L, Y_1/L < Y < Y_3/L; Y = Y_3/L, X_2/L < X < H/L$) boundary perfect thermal contact conditions taking into account liquid evaporation were accepted for thermal conduction equation, besides second-type boundary conditions taking into account vapors blow-in on border were assumed for thermal convection, diffusion and Poisson equations;

on axis of symmetry and boundaries ($Y = 0, Y = 1, 0 < X < H/L; X = H/L, 0 < Y < 1; Y = Y_3/L, X_1/L < X < X_2/L$) conditions of equal to zero gradients of corresponding functions were accepted for all equations.

The scale magnitudes were used to transfer dimensionless variables: L is characteristic size of solution area, m; V_m is scale of convection rate of fuel vapors nearby liquid surface, m/s; t_m is time scale, s ($t_m = 5$ s); T_m is temperature scale, K ($T_m = 1000$ K). Formulas for V_m, W_{cr}, W_o and dimensionless complexes are presented in papers [10–12].

The volume fractions of vapor and gas components in mixture were calculated from it mass concentrations according to the following expressions:

$$\varphi_4 = \frac{C_g/\rho_4(T)}{C_g/\rho_4(T) + C_o/\rho_1(T)}, \quad \varphi_1 + \varphi_4 = 1. \quad (8)$$

Thermophysical characteristics of gas-vapor mixture as heterogeneous system were calculated according to the formulas:

$$\lambda_5(T) = \lambda_1(T)\varphi_1 + \lambda_4(T)\varphi_4, \quad C_5(T) = C_1(T)\varphi_1 + C_4(T)\varphi_4, \quad \rho_5(T) = \rho_1(T)\varphi_1 + \rho_4(T)\varphi_4. \quad (9)$$

Size of fuel vapor gap between particle and liquid were determined at algorithm given in the paper [11].

4. Solution method

The solution algorithm of Eqs. (1)–(7) was similar to one used in papers [10–12]. This system of equations with initial and boundary conditions was solved by the finite difference method. The equations of elliptic type (1) and (2) were solved by the alternating directions method. The locally-one-dimensional method was applied to the solution of difference analogues for Eqs. (3)–(7). Nonlinear difference analogues of differential equations were solved by iteration method. The sweep method using the implicit four-dot difference scheme was applied to solution of one-dimensional difference equations.

The reliability of numerical research results was determined by the verification of difference scheme conservation. The error of the energy conservation law in the field of the solution area did not exceed 2.5%.

5. Results and discussion

Numerical investigations were carried out at the following values of process parameters: $\Theta_0 = 0.3$, $\Theta_p = 1$, $Q_o = 45 \cdot 10^6$ J/kg, $E = 130 \cdot 10^3$ J/mol, $k_0 = 7 \cdot 10^6$ s⁻¹, $Q_{cr} = 205 \cdot 10^3$ J/kg, $\beta = 0.009$ K⁻¹. Thermophysical characteristics of gasoline and its vapors, steel particle, air and water vapors

Table 1. Dimensionless ignition delay time at the system “hot particle – gasoline – air” versus dimensionless initial particle temperature Θ_p .

Θ_p	1.000	0.975	0.950	0.925	0.900	0.875	0.850
τ_d^*	0.309	0.344	0.394	0.463	0.569	0.643	no ignition
τ_d^{**}	0.287	0.306	0.370	0.426	0.506	0.608	no ignition
$\Delta, \%$	7.12	11.04	6.09	7.99	11.07	5.44	–

τ_d^* is dimensionless ignition delay time without taking into account the dependence of thermophysical characteristics on temperature [11];

τ_d^{**} is dimensionless ignition delay time at the taking into account the dependence of thermophysical characteristics on temperature;

Δ is deviation ($\Delta = (\tau_d^* - \tau_d^{**}) / \tau_d^* \cdot 100$), %.

Table 2. Dimensionless ignition delay time at the system “hot particle – gasoline – air” versus dimensionless initial particle temperature Θ_p .

Θ_p	2.000	1.900	1.800	1.700	1.600	1.500	1.250	1.000
τ_d^{**}	0.108	0.123	0.146	0.177	0.182	0.203	0.265	0.286
τ_d^{***}	0.083	0.104	0.130	0.161	0.174	–	–	–
$\Delta, \%$	23.15	15.44	10.96	9.04	4.39	–	–	–

τ_d^{**} is dimensionless ignition delay time without taking into account the particle material crystallization;

τ_d^{***} is dimensionless ignition delay time at the taking into account the particle material crystallization;

Δ is deviation ($\Delta = (\tau_d^{**} - \tau_d^{***}) / \tau_d^{**} \cdot 100$), %.

depending on temperature were chosen similarly to [10, 12]. Results of theoretical investigations are presented at $T_m = 1000 \text{ K}$, $L = 20 \cdot 10^{-3} \text{ m}$, $H = 10 \cdot 10^{-3} \text{ m}$, $L_p = 10^{-3} \text{ m}$, $H_p = 4 \cdot 10^{-3} \text{ m}$.

Numerical values of dimensionless ignition delay time τ_d^* versus dimensionless initial particle temperature Θ_p are presented in the Table 1. The analysis of ignition delay time shows that heat and mass transfer processes at system (Fig. 1) are implemented with less τ_d at increase of initial particle temperature. It can be explained by the increase of heat transfer rates from hot particle to liquid fuel and air. At this conditions temperature of gas-vapor mixture near particle increases. Accordingly probability of mixture ignition also increases.

It is significant that maximum deviation of τ_d^{**} and τ_d^* [11] is not more than 11%. The relatively small numerical values Δ (Table 1) can be explained by no significant change of thermophysical characteristics for substances at temperature interval ($\Theta_p = 1-2$). This result confirms relevancy of using for analysis of investigated process of mathematical model with assumption $\lambda = \text{const}$, $C = \text{const}$, $\rho = \text{const}$ for substances [11].

Welding and cutting of metal construction are often accompanied by particle formation at molten state. It can be supposed that energy transfer by phase changes (crystallization of hot particle material) is significant when particle interconnected with combustible liquid. Values of dimensionless ignition delay time τ_d^{**} versus dimensionless initial temperature Θ_p of hot particle are presented in the Table 2. The initial temperature of energy source is varied over the range including particle melting temperature. For steel particle dimensionless melting temperature is $\Theta_{cr} = 1.5$.

It is obvious (Table 2) that ignition delay time τ_d^{**} is significantly decreased in comparison with τ_d^{***} at initial particle temperature more than Θ_{cr} . It result can be explained by the additional heat release due to the crystallization of metal and consequently the acceleration of physical and chemical processes within the system (Fig. 1).

According to the Table 2 values of Δ are significantly increased at Θ_p that exceed particle melting temperature ($\Theta_p > 1.9$). However at Θ_p less than 1.6 the crystallization process of the particle negligently influence on numerical results of researches (Table 2). By this factor can be neglected at these temperatures.

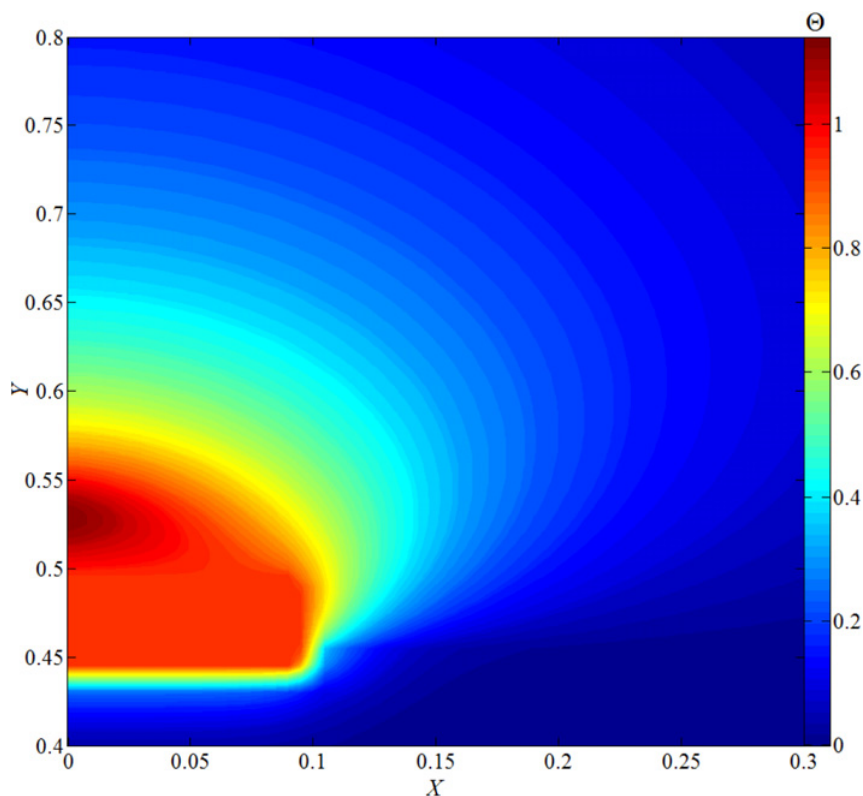


Figure 2. Dimensionless isotherms Θ at the system “hot particle – gasoline – air” at ignition moment ($\tau_d = 0.286$).

Numerical research results allow drawing a conclusion that model [7] of solid condensed substance ignition by massive energy source (hot plate) can not be used at analysis of ignition by single hot particle. It is due to the fact that small-size particle have limited heat content. Such particle is strongly cooled at immersion in liquid. Consequently temperature of particle surfaces and heat flow in evaporation zone strongly decrease. The ignition process at these conditions is often transient. Therefore ignition delay time of liquid by heated single particle is significantly limited. It can not increase 1 s in contrast to values of analogue characteristic (more than 10 s) for solid condensed substances [7] by heated massive energy source (hot plate).

The main peculiarities of investigated process are endothermic phase change at evaporation of liquid fuel and exothermic phase change at crystallization of hot particle material unlike to ignition process of solid fuel by single particle. Therefore methods, algorithms and models used at numerical investigation of powders and solid fuels ignition [7] can not be effective for research of liquid fuels ignition.

Distributions of Θ and C_f at the system “hot particle – gasoline – air” at $\Theta_p = 1$, $H_p^* = 0.2$, $L_p^* = 0.05$ (at ignition moment) graphically illustrated in Figs. 2 and 3.

Isotherms (Θ) are presented in Fig. 2. It is shown that the cooling of the particle occurs from all its borders. Due to the fact the ignition of gas-vapor mixture realizes at small sizes gas area over particle ($X = 0, 0.5 < Y < 0.55$). Obtained result can be explained by specific character of investigated process. Endothermic effect of phase exchange of combustible liquid evaporation is the reason of vapor temperature on the boundary “liquid – air” is not enough to ignite gas-vapor mixture. Ignition begins possible only after the additional heating fuel vapors while its moving nearby the side edges

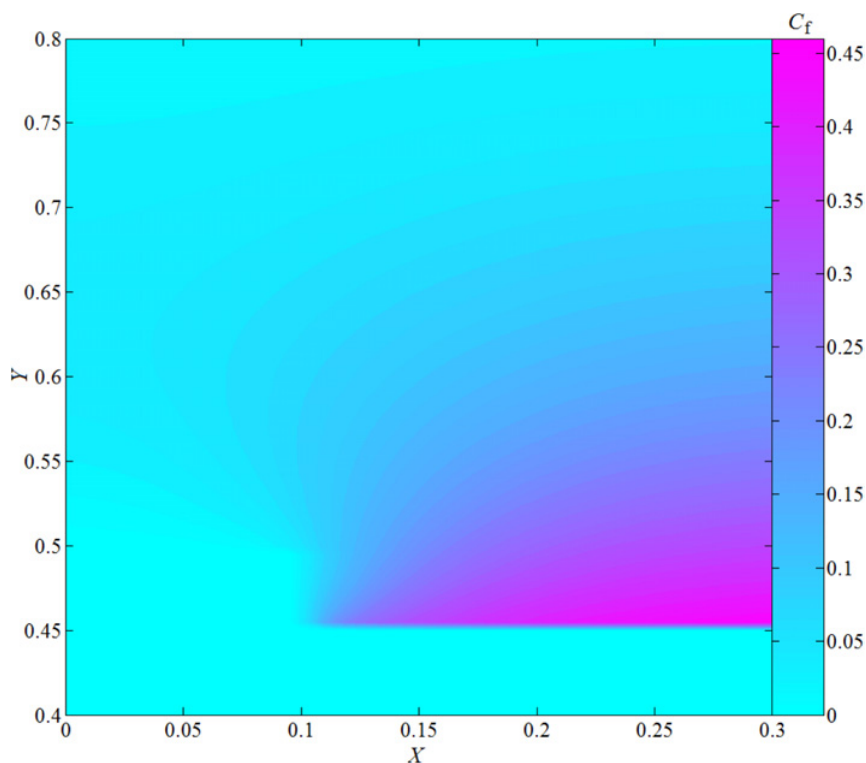


Figure 3. Distribution of fuel concentration C_f at the system “hot particle – gasoline – air” at ignition moment ($\tau_d = 0.286$).

particle. This is the reason of significant heterogeneousness of temperatures (Fig. 2) and fuel vapors concentration (Fig. 3) which is observed within system (Fig. 1).

It was established (Figure 3) that local maximum of fuel concentration C_f locates nearby the evaporation boundary ($0.1 < X < 0.4$, $Y = 0.45$). Fuel concentration decreases at vapor moving from liquid surface to gas area. It is caused by the most part of fuel vapor enter the air nearby hot particle. The fluxes of heated vapors unite while reaching the upper side of the particle. Therefore C_f is increased in this gas area. At the ignition moment the rate of combustible vapors oxidation raises rapidly and its concentration decreases near energy source vicinity (Fig. 3).

Analysis of Figs. 2 and 3 shows that areas of significant changes of main parameters for investigated process have small sizes relative to energy source sizes. It factor and other factors (high temperature and small sizes of energy source, high rates of physical and chemical processes) complicate experiment investigation of liquid ignition processes at concerned statement (Fig. 1).

It is obvious that determination of kinetics for ignition of liquid by single hot particle realizes with difficult factors which are no characteristic for ignition of combustible liquid drops on hot surface [15]. Ignition delay time at concerned system depends on sizes and heat content of particle. Correspondingly values of activation energy E and preexponential factor k_0 also change.

6. Conclusions

Numerical research results of interconnected heat and mass transfer processes at the ignition of liquid fuel by heated till high temperatures particle allow drawing a conclusion about obvious expressed

mechanism of gas-phase ignition for combustible liquids. Oxidation reaction for fuel vapor begins at the significant increase of mixture temperature over the fuel evaporation temperature. Endothermic phase change at evaporation of liquid fuel reduces rates of heat and mass transfer in a system “hot particle – gasoline – air”. The highest rates of heat and mass transfer processes are possible at temperature of hot particle higher than melting temperature of its material due to exothermic phase change at crystallization of hot particle material.

Mathematical model and investigated regularities can be useful at development of power effective ignition system due to heat transfer enhancement at local energy sources interaction with various combustible liquid substances.

The reported study was supported by State task “Nauka” (code of the federal target scientific and technical program No. 2.1321.2014).

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