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The Numerical Modelling of Burning the Liquid Fuel Drop Performed by the Finite Element Method

It was proposed a mathematical model for burning the liquid fuel drop in a hot oxidizing environment. The model was numerically solved by the finite element method. The droplet ignition periods were calculated as a function of ambient temperature, oxygen concentration, initial droplet diameter and activation energy.

Keywords: *mathematical model, liquid, fuel drop, finite element method*

1. The physical model

The object of this analysis is the liquid fuel droplet gradually subjected to the action of hot, gaseous and exogenous medium. The fuel vapours at the surface of drop diffuse to the environment and from the environment to the surface of drop diffuse the oxygen. In each point of the area surrounding the drop in which the fuel and oxygen vapour concentrations are non-zero, a chemical reaction is produced at a rate determined by Arrhenius' reaction, generating the heat release, the fuel and oxygen consumption as well as the appearance of burning products. In a certain point of which position depends on the heat balance of the system, the temperature of gas increases reaching the ignition point. We propose the following working assumptions:

- the fuel droplet considered has a sphere symmetry according to the assumption that there is no relative motion between the droplet and the gas, as well as the free convection is negligible;
- the heat transfer is made only by conduction;
- the pressure is the same all over the droplet medium and constant in time;
- the temperature of droplet surface is equal to the boiling temperature of the liquid at the given pressure;

- all the components of the gaseous medium satisfy the equation of perfect gas state;
- the chemical reaction is a second-order reaction with a rate established by Arrhenius'law.

2. The mathematical model

The processes developed in a gaseous atmosphere surrounding the droplet are described by the set of equations for the energy conservation and for the components. This set is formed of the equation of non-steady heat conduction including the flux term resulted from the chemical reaction and other four non-steady equations of mass. Taking into account the heat dissipation and including the flux terms for vapours of fuel, oxygen, nitrogen and burning products, we can write:

$$\frac{\partial T}{\partial t} = \frac{1}{r^2 C_p \rho} \frac{\partial}{\partial r} \left(\lambda r^2 \frac{\partial T}{\partial r} \right) + \frac{Q}{C_p \rho} A C_1 C_2 \sqrt{p} \exp\left(-\frac{E}{RT}\right) \quad (1)$$

$$\frac{\partial C_i}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\frac{D_i r^2}{T} \frac{\partial C_i T}{\partial r} \right) + b_i A C_1 C_2 \sqrt{T} \exp\left(-\frac{E}{RT}\right) \quad (2)$$

where:

C – concentration of component i = 1,2,3,4 – refers to fuel, oxygen, nitrogen and burning gases;

D – mass diffusion coefficient (m²/s);

λ – coefficient of thermal conductivity;

A – pre-exponential constant (m³/kg s deg^{1/2});

ρ – density (kg/m³);

b_i – stoichiometric coefficient for component i.

The indices used in the development of mathematical model:

c – liquid;

g – gas

k – droplet

N – normal conditions

p – fuel;

s – droplet surface

w – boiling;

z – ignition;

0 – initial parameters;

1 – fuel;

2 – oxygen;

3 – nitrogen;

4 – burning gases;

∞ – parameters of a gas element at a long

distance to the droplet.

The existing conditions in the droplet are described by the equation of non-steady heat conduction:

$$\frac{\partial T}{\partial t} = \frac{1}{r^2 C_p \rho} \frac{\partial}{\partial r} \left(\lambda r^2 \frac{\partial T}{\partial r} \right) \quad (3)$$

The boundary conditions for the three above equations are the following:
-for $t = 0$

$$\begin{aligned} T(r,0) &= T_{k0} \text{ pentru } r \leq r_k \\ T(r,0) &= T_0 \text{ pentru } r > r_k \\ C_1(r,0) &= 0 \\ C_2(r,0) &= C_{2,0} = g_{2,0} \frac{M_2 T_N p_0}{22,4 T_0 p_N} \\ C_3(r,0) &= C_{3,0} = g_{3,0} \frac{M_3 T_N p_0}{22,4 T_0 p_N} \text{ pentru } r > r_k \\ C_4(r,0) &= 0. \end{aligned} \quad (4)$$

where:

M_i - is the molar mass of the i component [kg /Kmol];

- for $t > 0$

$$\begin{aligned} \frac{\partial T}{\partial r} &= 0 \text{ pentru } r = 0; \\ T(r_k, t) &= T_w; \\ C_1(r_k, t) &= \frac{M_1 T_N p_0}{22,4 T_w p_N}; \\ C_2(r_k, t) &= 0; \\ C_3(r_k, t) &= 0; \quad C_4(r_k, t) = 0; \\ T(r, t) &= T; \quad C_1(r, t) = 0; \\ C_2(r, t) &= C_{2,0}; \quad C_3(r, t) = C_{3,0}; \\ C_4(r, t) &= 0. \end{aligned} \quad (5)$$

Because of the non-linearity of the equations (1), (2) and (3) the analytical resolution of the problem is not possible and it is necessary the numerical resolution.

3. The resolution of heat conduction equation

The resolution of this problem is to find the unknown function T defined in V domain, according to the differential equation $F(T) = 0$. For the unidimensional case studied of the non-steady heat conduction, the equation is:

$$F(T) = \frac{1}{r^2 C_p \rho} \frac{\partial}{\partial r} (\lambda r^2 \frac{\partial T}{\partial r}) - \frac{\partial T}{\partial t} + \frac{Q}{C_p \rho} Z = 0; \quad (6)$$

where:

Z – is the part of source (the source element);

$$Z_{(r,t)} = AC_1 C_2 \sqrt{T} \exp\left(\frac{E}{RT}\right). \quad (7)$$

For the finite element method, the function T is expressed inside of a finite element "I" of V domain by its values in the nodal points $\{T\}^I$ and the functions given by participation $[N]^I$ named the shape functions:

$$\{T\}^I; \quad (8) \quad T = [N]^I$$

where:

N = is the shape function of spatial element.

For the problem studied, the non-steady unidimensional function with the division of space T (r,t) in the element I has the form:

$$T(r,t) = \sum_{i=1}^m N_i^I(r) T_i^I(t); \quad (9)$$

where:

m – number of nodes (points) in the element.

For the problem studied $m = 2$. The above presentation of the function is an approximation and thus:

$$F(T_{(r,t)}) = R \neq 0. \quad (10)$$

The accurate resolution of this problem will be the resolution which minimizes the residue of R equation in all the points of V domain.

4. Test results for marine Diesel fuel

To estimate the values of interest, namely, the dependence of delay time of ignition on the initial diameter of droplet, the dependence of delay time of droplet ignition on the ambient temperature as well as the dependence of delay time of ignition on the activation energy value and on the pre-exponential constant mainly for the calculation of the values and the parameters specific to marine Diesel DMA light fuel (marine fuel):

$$\begin{aligned} \rho_c &= 890 \text{ [kg/ m}^3\text{]}; \\ \lambda_c &= 1,163 (0,12993 - 0,000025.T) \text{ [J/ m s K]}; \\ C_{pc} &= 4186,8. (-0,02144 + 0,00149. T) \text{ [J/kg K]}; \\ Q &= 4192.10^7 \text{ [J / kg]}; \\ T_w &= 353,26 \text{ [K]}; \\ L &= 3,94. 10^5 \text{ [J/ kg]}. \end{aligned}$$

The constants of diffusion have been calculated according to the relation:

$$D_i = D_0 (T_i / 273)^2, \quad (4)$$

where the values of diffusion D_0 constants "i" at the temperature 273 [K] are:

- for marine Diesel light fuel: $D_0 = 0.751 \cdot 10^{-5} \text{ [m}^2\text{/s]}$;
- for oxygen: $D_0 = 1.78 \cdot 10^{-5} \text{ [m}^2\text{/s]}$;
- for nitrogen: $D_0 = 1.8 \cdot 10^{-5} \text{ [m}^2\text{/s]}$.

The diffusion constant for burning gases was calculated as a weighted average between the diffusion constants of CO_2 for which $D_0 = 1.39 \times 10^{-5} \text{ (m}^2\text{/s)}$ and the water vapours $D_0 = 2.0 \times 10^{-5} \text{ [m}^2\text{/s]}$ by the relation:

$$D_{0,sp} = g_{CO_2} \cdot D_{0CO_2} + g_{H_2O} \cdot D_{0H_2O}; \quad (5)$$

Taking $g_{CO_2} = 0,83$ and $g_{H_2O} = 0,17$, we have: $D_{0,sp} = 1,49 \times 10^{-5} \text{ [m}^2\text{/s]}$.

For calculation we take into account the variation of conductivity coefficient λ_g and the specific heat coefficient C_{pg} related to the temperature and the gas

composition in the ignition medium. It was supposed that at the droplet surface the temperature is equal with the liquid boiling temperature and the concentration of fuel vapours is constant and equal with the concentration of saturated vapours.

5. The dependence of delay time of ignition on the activation energy value and on the pre-exponential constant

The estimated delay time of droplet ignition mainly depends on the activation energy value E and on the pre-exponential constant A , appearing within the flux that mark the rate of oxidation reaction. These values are difficult to determine for the most fuels used. In Figure 1 and Figure 2 it is presented the dependence of delay time of ignition the DMA light fuel droplet with its initial diameter $d_0 = 500$ [μm] and the initial temperature $T_{p0} = 300$ [K] placed in the air with $t_a = 1000$ [K] on the activation energy and the pre-exponential constant.

The delay time of ignition the DMA light fuel droplet is inversely proportional with the value of pre-exponential constant, the variation ratios being different depending on the activation energy value; thus, the three times increment of the pre-exponential constant value, for the same characteristically values of environment, droplet and activation energy, led to the reduction of delay time value of ignition, from 1.6 to 4.5 times.

As the delay times of ignition experimentally determined, under the same conditions, have different values (from a few milliseconds to 2.5 seconds) the estimation of real values of E and A , on practical data, and of the curves in Figs.1 and 2, is relative. The values of the activation energy and the pre-exponential constant were estimated in the following way:

- from the experimental data, they were adopted the values of critical diameter of light fuel droplet $d_{ocr} = 200$ μm at an ambient temperature of $T_0 = 1090$ [$^{\circ}\text{K}$];
- the value of the activation energy was chosen so that the ignition should be performed when the droplet evaporation was completed, $E = 41350$ (kJ/kmol);
- for the other calculations, they were adopted the data obtained at tests, so $E = 41350$ (kJ/kmol) and $A = 100$ ($\text{m}^3/\text{kg s K}^{1/2}$).

6. The dependence of delay time of droplet ignition on the ambient temperature

The calculations were made for a variable ambient temperature T_0 , from 800 to 1300 [$^{\circ}\text{K}$], for different initial parameters of the droplet and different shares of oxygen in the burning medium. The results have been presented in Figures 3 and 4 by the relation:

$$\lg \tau_z = f(1/T_0) . \quad (6)$$

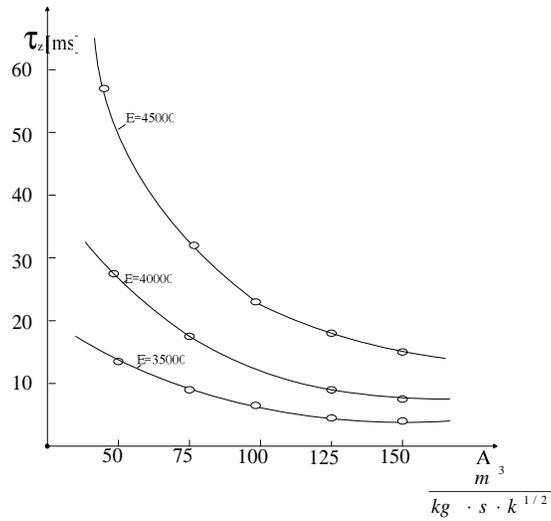


Figure 1. The dependence of delay time of ignition the marine DMB fuel droplet on the activation energy for different values of pre-exponential constants.

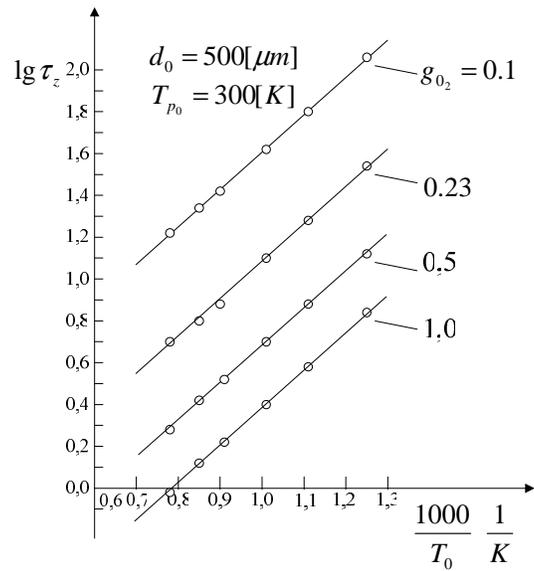


Figure 2. The dependence of delay time of ignition the marine DMB fuel droplet on the pre-exponential constant for different values of the activation energy

The curves represented in the figures are almost some straight lines, resulting that the delay time of fuel droplet ignition is an exponential function of ambient temperature.

The curves represented in the Figures 3 and 4 can be used for determining the constants A_z and E_z on the experimental data, with the relation:

$$\tau_z = A_z \exp(-E_z / R.T_0); \quad (7)$$

where: A_z and E_z are the conventional activation energy and the initiation energy of ignition.

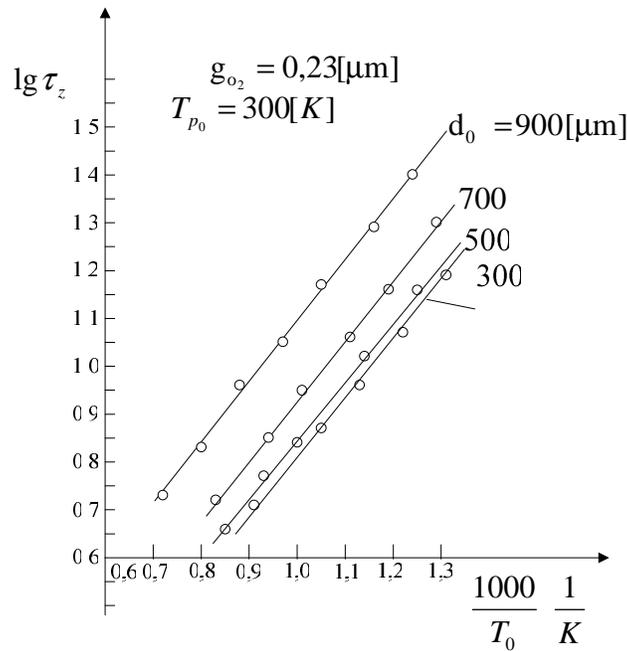


Figure 3. The dependence of delay time of ignition the marine DMB fuel droplet on the ambient temperature for different initial diameters.

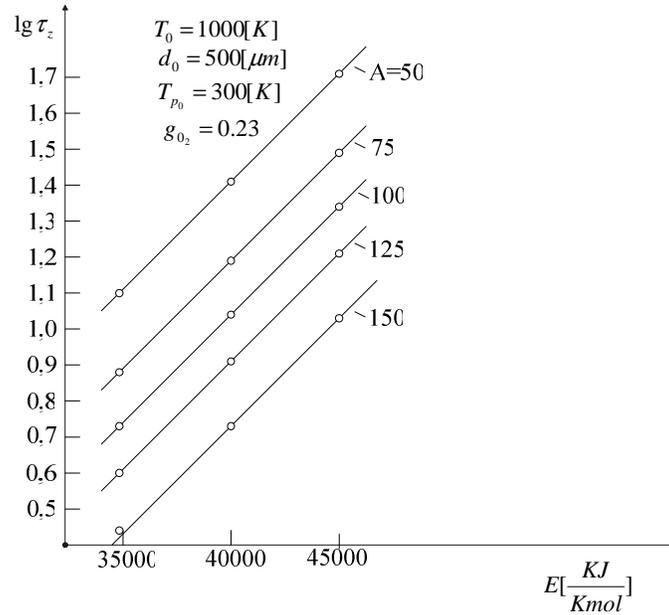


Figure 4. The dependence of delay time of ignition the marine DMB fuel droplet on the ambient temperature for different oxygen concentrations.

7. The dependence of burning time of droplet on the initial diameter

In Figure 5 it was represented the dependence of burning time of droplet at the ambient temperatures between 700 – 1100 [°K] for different initial diameters of droplet. It is obvious that the burning time is much reduced with the decrease of initial diameter of the droplet.

8. The dependence of burning time of volatile matters and of cenosphere

The dependence of burning time of volatile matters in the marine DMB fuel droplet for different initial diameters and temperatures of oxygen carrier medium is presented in Figure 6.

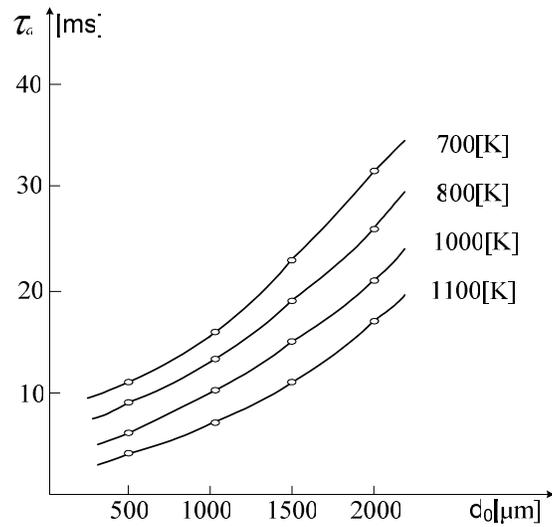


Figure 5. The dependence of delay time of ignition the marine DMB fuel droplet for different initial diameters and different ambient temperatures.

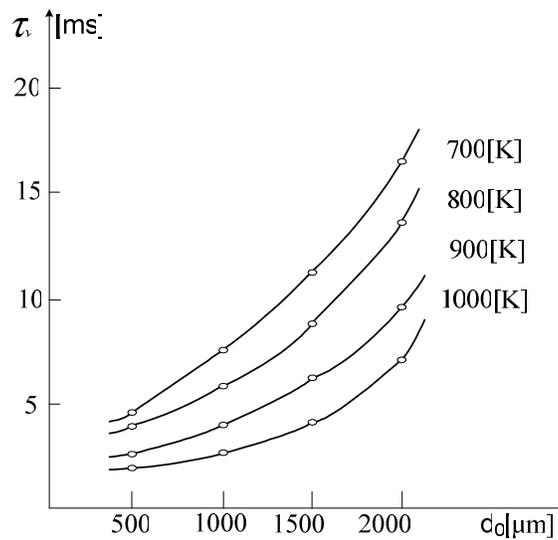


Figure 6. The dependence of burning time of volatile matters in the marine DMB fuel droplet for different initial diameters and temperatures of oxygen carrier medium

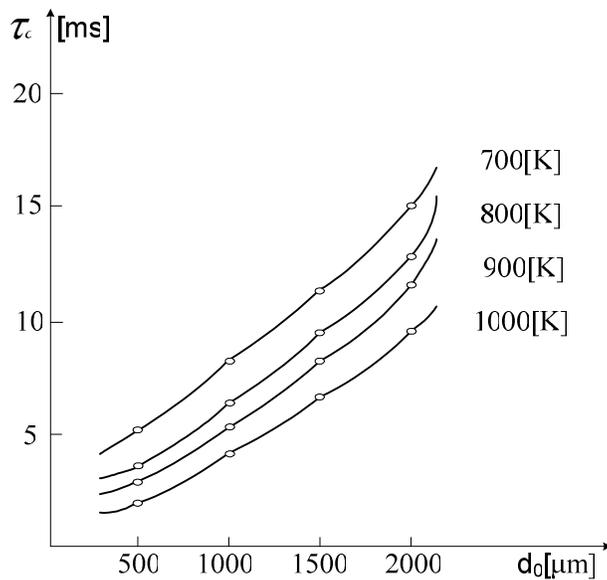


Figure 7. The dependence of burning time of cenosphere in the marine DMB fuel droplet for different initial diameters and temperatures of oxygen carrier medium

So, the burning time of volatile matters in the fuel droplet is much reduced with the decrease of initial diameter of the droplet. Figure 7 presents the dependence of burning time of cenosphere in the marine DMB fuel droplet for different initial diameters and ambient temperatures. It has been found that there is an obvious dependence of burning times, to the movement direction, with the decrease of burning droplet.

4. Conclusion

The calculations made related to the process of ignition a fuel droplet in hot oxygen medium, allow to draw the following conclusions:

- the delay time of fuel droplet ignition is an exponential function of the ambient temperature; the activation energy of ignition (conventional ignition energy) hasn't a constant value, it depends on the oxygen concentration in the medium and on the initial diameter of the droplet;
- the delay time of ignition depends on the initial diameter of the droplet, specially, for low relative temperatures of the medium and droplets of average initial diameter;

- the delay time of ignition depends on the oxygen concentration, specially, for low temperatures and low oxygen concentration;
- the life time of the droplet reduces with the increase of the ambient temperature and the oxygen concentration;
- the life time of the droplet reduces with the decrease of its initial diameter;
- it hasn't been found a dependence of the delay time of ignition on the initial temperature of the droplet, which is a result of the assumption that at the droplet surface it is considered the liquid boiling temperature. It hasn't been found an important influence of the initial temperature of the droplet on the value of critical diameter;
- disregard for the influence of heat diffusion on the mass transfer process leads to a low variation of the delay time of fuel droplet ignition (< 1%).

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