

**Askarova A.S., Bolegenova S.A., Berezovskaya I.E.\* , Laptev V.,  
Vorobieva O.D., Zhanzhienov A.E., Karymsakova L.I., Iliyeva M.M.**

Al-Farabi Kazakh National University,  
Kazakhstan, Almaty, \*e-mail: Yryna.Berezovskaya@kaznu.kz

## **INVESTIGATION OF TURBULENT HEAT AND MASS TRANSFER IN COMBUSTION OF THE LIQUID FUEL**

Conducted research of inflammation of the hexadecane depending on the level of pressure in the combustion chamber under given primary conditions. In the process of work, pressure was increased till 200 bars for choosing optimum characteristics of combustion. In the result of work obtained schedules of distribution of the maximum temperature, maximum concentration of the carbon dioxide and water steam, time of inflammation from the pressure in the combustion chamber. Individually provided distribution of the temperature fields at the moment of inflammation and temperature at the moment of active fuel combustion depending on the pressure in the combustion chamber. Based on the obtained results and schedules, chosen optimum pressure equal to 170 bars, when noticed inflammation with the time of delay equal to 0.8 ms, temperature in the combustion chamber is reaching 2697 K, and also discharging relatively low concentration of the carbon dioxide 0.186 g/g.

**Key words:** inflammation, liquid fuel, pressure, computational research, combustion chamber.

Аскарова Ә.С., Бөлегенова С.А., Березовская И.Э.\* , Лаптев В.,  
Воробьева О.Д., Жанжиенов А.Е., Қарымсақова Л.И., Илиева М.М.

Әл-Фараби атындағы Қазақ ұлттық университеті,  
Қазақстан, Алматы қ., \*e-mail: Yryna.Berezovskaya@kaznu.kz

### **Сұйық отынды жағу кезінде турбулентті жылу-масса алмасу процесстерін зерттеу**

Берілген бастап қыжағдайлар дажану камерасының кеңістігіндегі қысымның мәніне байланысты гексадеканның тұтануына зерттеу жүргізілді. Жұмыс барысында жанудың оңтайлы сипаттамаларын таңдау үшін қысымды 200 барға дейін өсірдік. Жұмыс нәтижесінде ең жоғары температураны бөлу кестесі, көмірқышқыл газы мен су буының ең жоғары концентрациясы, жану камерасындағы қысымнан жану уақыты алынды. Жану камерасының кеңістігіндегі қысымға байланысты отынның белсенді жану сәтіндегі температура және жану сәтіндегі температура өрістерінің таралуы жеке көрсетілген. Жану камерасының кеңістігіндегі қысымға байланысты отынның белсенді жану сәтіндегі температура және жану сәтіндегі температура өрістерінің таралуы жеке көрсетілген. Алынған нәтижелер мен графиктердің негізінде 170 барға тең оңтайлы қысым таңдап алынды, ол кезде кідіріс уақыты 0,8 мс тең, жану камерасындағы температура 2697 К жетеді және көмірқышқыл газының салыстырмалы жоғары емес концентрациясы 0,186 г/г бөлінеді.

**Түйін сөздер:** тұтану, сұйық отын, қысым, сандық зерттеу, жану камерасы.

Аскарова А.С., Болегенова С.А., Березовская И.Э.\* , Лаптев В.,  
Воробьева О.Д., Жанжиенов А.Е., Карымсакова Л.И., Илиева М.М.

Казахский национальный университет имени аль-Фараби,  
Казахстан, г. Алматы, \*e-mail: Yryna.Berezovskaya@kaznu.kz

### **Исследование процессов турбулентного теплопереноса при сжигании жидкого топлива**

Проведены исследования воспламенения гексадекана в зависимости от значения давления в пространстве камеры сгорания при заданных начальных условиях. В процессе работы давление увеличивали до 200 бар для выбора оптимальных характеристик горения. В результате работы получены графики распределения максимальной температуры, максимальной концентрации углекислого газа и паров воды, времени воспламенения от давления в камере сгорания. Отдельно представлены распределения полей температуры в момент воспламенения и температуры в момент активного сгорания топлива в зависимости от давления в пространстве камеры сгорания. На основе полученных результатов и графиков выбрано оптимальное давление, равное 170 бар, при котором наблюдается воспламенение с временем задержки равным 0,8 мс, температура в камере сгорания достигает 2697 К и выделяется относительно невысокая концентрация углекислого газа 0,186 г/г.

**Ключевые слова:** воспламенение, жидкое топливо, давление, численное исследование, камера сгорания.

#### **Introduction**

Importance of this work is associated with the fact that major sources of energy used within the world are non renewable. According to the statistics done by International Energy Agency in 2010, approximately 90% of the whole energy produced by humanity was produced by combustion of fuel and bio fuel [1]. As per the forecasts of the Energy research and development Administration (USA), this portion will not reduce till the level below 80% till 2040 in case of synchronous increase of energy consumption level to 56% during 2010 to 2040 [2]. Such a long and intensive usage of the limited resources will bring to: 1) gradual depletion of the resources; 2) increase of concentration of hazardous substances in the atmosphere. Consequently, nowadays we shall search for the ways of optimal usage of the resources.

It is known that in the heating chambers of the power stations burning solid, fluid and gaseous fuel, while modern heating units achieved large capacities and high level of improvement as per provision of maximum combustion. One of the facts against usage of the coal is high level of hazardous emissions of the combustion products. However new technologies in our country have been developed and still being developed [3-8].

Engines of internal combustion are using the process of burning gases or vaporous and fluid fuel and forming energy basis of aviation and traffic transportation. Burning of the fluid fuel differs by several specifics as leakage of chemical charges

under dynamic and heat impact of the chemicals, intensive mass transfer during change of phase, also by depending of the process parameters from thermal dynamic state of the system and from its structural characteristics [9-10].

In this work, we are researching inflammation of the fluid fuel under high pressure. The researched processes are described by equations of: continuity, impulse, energy,  $k$ - $\epsilon$  model of turbulence [9]. Simulation exercise means research of the processes of diffusion, inflammation and burn of the hexadecane in the cylindrical combustion chamber under high pressure for choosing optimal parameters of those processes. Computer modeling of the process of burning of energy fuel is allowing to conduct experiment with less expenses, with higher quality and more safely. At the moment existing several efficient models of burning in the combustion chamber which providing possibility of calculations of most parameters of the process: from thermal fields and distribution of velocity till modeling emission characteristics. [11-19].

#### **Model of evaporation, burning and collision of droplets**

Mathematic model which can explain above mentioned physical chemical processes includes equations [9], and ending up with statement of the equation of evaporation. This equation contains distribution of the probability density function  $f$ , which has ten independent variables additionally to time: three positions of droplets by  $x$ , three velocity

components  $v$ , radius  $r$ , temperature  $T_d$  (accepted as equal within the droplet limits), deviation from the sphere  $y$  and changing along with the deviation time  $dy/dt = \dot{y}$ .

Element of the fluid scope  $\theta$ , is defined as:

$$\theta = \int f 4 / 3 \pi r^3 dv dr dT_d dy d\dot{y}. \quad (1)$$

Macroscopic density of the fluid phase  $\rho'_l$ , is identified as:

$$\rho'_l = \rho_d \theta, \quad (2)$$

where  $\rho_d$  is a constant term, microscopic density of the fluid phase which may still be compared with gas density, as proportion of  $\rho_d$  to  $\rho$  is high. Change of  $f$  function can be achieved by resolving the equation of evaporation of fluid droplet:

$$\begin{aligned} \frac{\partial f}{\partial t} + \nabla_x(fv) + \nabla_v(fF) + \\ + \frac{\partial}{\partial r}(fR) + \frac{\partial}{\partial T_d}(fT_d) + \\ + \frac{\partial}{\partial y}(f\dot{y}) + \frac{\partial}{\partial \dot{y}}(f\dot{y}) = \dot{f}_{coll} + \dot{f}_{bu} \end{aligned} \quad (3)$$

Values  $\dot{f}_{coll}$ ,  $\dot{f}_{bu}$  – a resources resulting from collision and rupture of droplets. Critical parameter of impact  $b_{cr}$  is defined as:

$$\dot{f}_{bu} = \int f(x, v_1, r_1, T_{d1}, 1, \dot{y}_1, t) \dot{y}_1 B(v, r, T_d, y, \dot{y}, v_1, r_1, T_{d1}, \dot{y}_1, x, t) dv_1 dr_1 dT_{d1} d\dot{y}_1. \quad (6)$$

Radiuses of the droplets are subject to the quadratic distribution:

$$g(r) = \frac{1}{\bar{r}} e^{-r/\bar{r}}. \quad (7)$$

Sauter mid radius  $r_{32}$  is expressed with a formula:

$$r_{32} = 3\bar{r} = \frac{r_1}{\frac{7}{3} + \frac{1}{8} \frac{p_d r_1^3}{a(T_{d1})} \dot{y}_1^2}. \quad (8)$$

$$b_{cr}^2 = (r_1 + r_2)^2 \min(1.0, 2.4 f(y) / W_{el}),$$

$$\text{where } f(y) = y^3 - 2.4 y^2 + 2.7 y,$$

$$y = r_2 / r_1,$$

$$W_e = \rho_d |v_1 - v_2| r_1 / a(\bar{T}_d),$$

where  $r_1 \leq r_2$ ,  $\bar{T}_d = \frac{r_1^3 T_{d1} + r_2^3 T_{d2}}{r_1^3 + r_2^3}$ . Expression for the function of the frequency collision  $\sigma$  has following form:

$$\begin{aligned} \sigma = \frac{b_{cr}^2}{(r_1 + r_2)^2} \delta \left[ r - (r_1^3 + r_2^3)^{\frac{1}{3}} \right] \times \\ \times \delta \left[ v - \frac{r_1^3 v_1 + r_2^3 v_2}{r_1^3 + r_2^3} \right] \delta \left[ T_d - \frac{r_1^3 T_{d1} + r_2^3 T_{d2}}{r_1^3 + r_2^3} \right] \times \\ \times \delta(y - y_2) \delta(\dot{y} - \dot{y}_2) + \frac{2}{(r_1 + r_2)^2} \times \end{aligned} \quad (5)$$

$$\times \int_{b_{cr}}^{r_1+r_2} \left[ \delta(r-r_1) \delta(v-v'_1) \delta(T_d-T_{d1}) \delta(y-y_1) \delta(\dot{y}-\dot{y}_1) + \delta(r-r_2) \delta(v-v'_2) \delta(T_d-T_{d2}) \delta(y-y_2) \delta(\dot{y}-\dot{y}_2) \right] b db,$$

Source term resulting from rupture of the droplet,  $\dot{f}_{bu}$ , is defined as:

Velocity of the droplets also differs from the parental droplet with a velocity  $w$  and direction distributed randomly in the normal projection for the vector of relativistic velocity between parental droplet and gas. The value of  $w$  is being given in following formula:

$$w = 1 / 2 r_1 \dot{y}_1. \quad (9)$$

Expression for  $B$  has following form:

$$B = g(r)\delta(T_d - T_{d1})\delta(y)\delta(y)\frac{1}{2\pi}\int\delta[v - (v_1 + \omega\vec{n})]d\vec{n}. \quad (10)$$

Speeding up the  $\vec{F}$  droplet by means of aerodynamic resistance and gravitation power has following form:

$$\vec{F} = \frac{3}{8}\frac{\rho}{\rho_d}\frac{|u + u' - v|}{r}(u + u' - v)C_D + g. \quad (11)$$

Resistance ratio  $C_D$  is defined as:

$$C_D = \frac{24}{\text{Re}_d}(1 + 1/6\text{Re}_d^{2/3}) \text{Re}_d < 1000, \quad (12)$$

$$0.424, \text{Re}_d > 1000,$$

where  $\text{Re}_d = \frac{2\rho|u + u' - v|r}{\mu_{air}(\hat{T})}$ ,  $\hat{T} = \frac{T + 2T_d}{3}$ . It is considered that each component  $u'$  is taken from the Gaussian distribution with medium quadrant deviation  $2/3 k$ . Consequently, accepting:

$$G(\vec{u}') = (4/3\pi\kappa)^{-3/2} \exp\{-3|\vec{u}'|^2/4\kappa\}. \quad (13)$$

Level of change of the droplet radius  $R$ :

$$R = -\frac{(\rho D)_{air}(\hat{T})}{2\rho_d r} \frac{Y_1^* - Y_1}{1 - Y_1^*} Sh_d, \quad (14)$$

where  $Sh_d$  is Sherwood number for mass transfer,  $Y_1^*$  is mass fraction of the fuel vapors at the surface of the droplets,  $Y_1 = \rho_1/\rho$ ,  $(\rho D)_{air}(\hat{T})$  is ratio of the fuel vapor diffusion in the air.

Sherwood number is identified as:

$$Sh_d = (2.0 + 0.6\text{Re}_d^{1/2} Sc_d^{1/2}) \frac{\ln(1 + B_d)}{B_d}, \quad (15)$$

where  $Sc_d = \frac{\mu_{air}(\hat{T})}{\rho D_{air}(\hat{T})}$  и  $B_d = \frac{Y_1^* - Y_1}{1 - Y_1^*}$ . Surface mass fraction  $Y_1^*$  is obtained from the following equation:

$$Y_1^*(T_d) = \frac{W_1}{W_1 + W_0(\frac{p}{p_0(T_d)} - 1)}, \quad (16)$$

where  $W_0$  is local medium molar mass for all types of fuel vapors, a  $p_0(T_d)$  is a balanced pressure of fuel vapors under the temperature  $T_d$ . For the vapor diffusion in the air, using empiric correlation:

$$(\rho D)_{air}(T) = D_1 T^{D_2},$$

where  $D_1$  and  $D_2$  are constants.

Change of the droplet temperature is explained with equation of the energy balance:

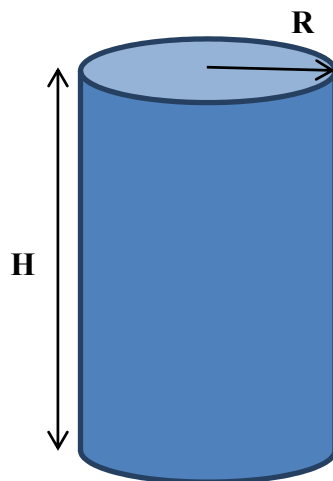
$$\rho_d \frac{4}{3}\pi r^3 c_1 \dot{T}_d - \rho_d 4\pi r^2 RL(T_d) = 4\pi r^2 Q_d, \quad (17)$$

where  $c_1$  is specific mass of fluid,  $L(T_d)$  is specific heat of evaporation, and  $Q_d$  is thermal conductivity at the surface of the droplet in unit volume [13-18]. In this work, kinetics is being given by means of the global model of chemical reactions [19].

### Formulation of the task about combustion of the fluid fuel

Burning occurs in the combustion chamber of 15 cm height and with 2 meter radius (Fig.1). Temperature in the combustion chamber is equal to 900 K, temperature of the walls of the combustion chamber – 353 K. The chamber is divided into 600 control cells. In the center of the lower base of the chamber located nozzle of the injector of  $2 \cdot 10^{-4} \text{ cm}^2$ , through which into chamber flowing the researching fuel – hexadecane ( $\text{C}_{16}\text{H}_{34}$ ), its temperature at the moment of injection is equal to 300 K. Hexadecane – is acyclic saturated hydrocarbon of normal structure; colorless liquid,  $T_{melt} = 291.35 \text{ K}$ ,  $T_{boil} = 559.95 \text{ K}$ ,  $T_{inflamm} = 408.15 \text{ K}$ , density  $0.7751 \text{ g/cm}^3$  (in fluid state, under 295.15 K, in respect of water under 277.15 K); not soluble in water, soluble in diethyl ester, ethanol and acetone [20].

Another name is cetane. Application: a template for assessing the quality (cetane number) of the diesel fuel. Cetane number – indicator of self combustion of the fuel which is equal to such content of cetane in  $\alpha$ -methyl naphthalene, when self combustion of this admixture and tested fuel is equal [20].



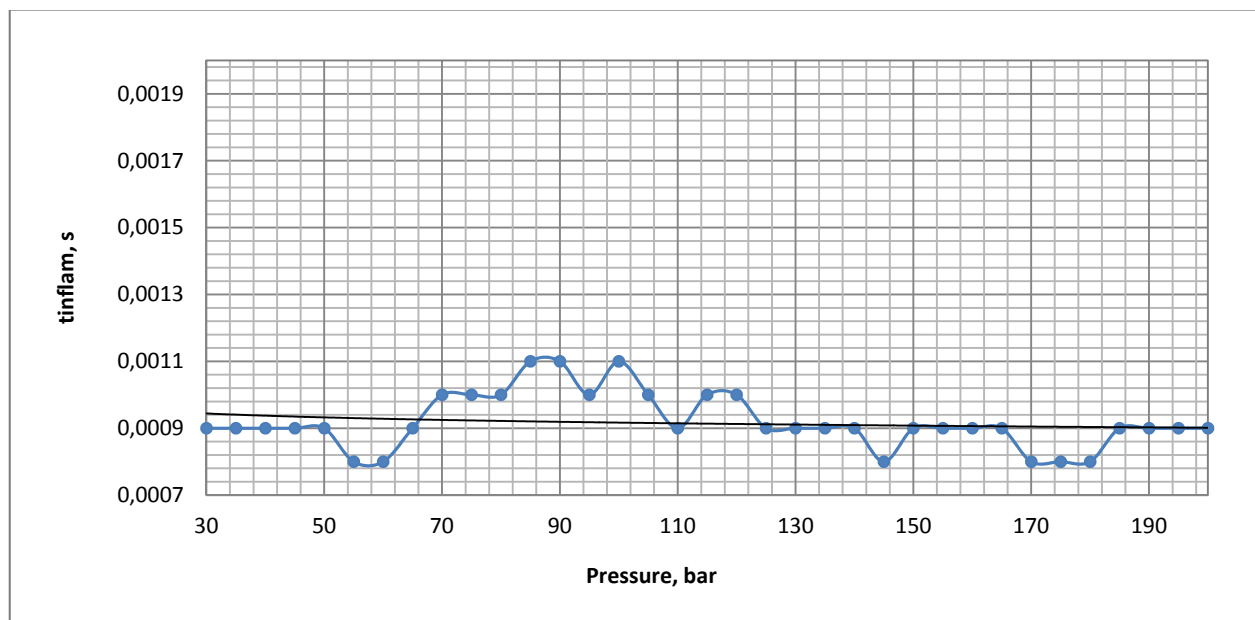
**Figure 1** – Visual appearance of the combustion chamber

Most important factor during mathematic modeling of the processes of combustion chamber is searching most rational values of the constructive and performance processes which allow to achieve maximum fuel efficiency during reduction of the emission of the hazardous substances.

## Results of the numerical studies

In this work we've been increasing the pressure in the combustion chamber from 30 to 200 bars. Liquid fuel is being injected through nozzle. It is located in the center of the chamber base; after injection the fluid is evaporating and burning occurs in the gaseous phase. Hexadecane was used as fuel. Chemical kinetics of burn of the hexadecane:  $2C_{16}H_{34} + 49O_2 \rightarrow 32CO_2 + 34H_2O$ . Below given dependence of the burning period (Fig.2), maximum temperature (Fig.3), concentration of the carbon dioxide (Fig.4), and concentration of the water vapors (Fig.5) from the pressure in the combustion chamber.

At the Fig.2 shown dependence of the time of inflammation from pressure. Least time of inflammation or time of delay is equal to 0.8 ms (when  $p = 55; 60; 145; 170; 175; 180$  bar), and the highest – 1.1 ms (when  $p=85; 90; 100$  bar). Shall note that  $t_{inflamm}$  approximately is equal to 1 ms, and consequently such increase of pressure in the combustion chamber is not having high impact to its value.



**Figure 2** – Dependence of the time of inflammation from pressure in the combustion chamber

At the Fig.3 shown dependence of the maximum temperature in the combustion chamber from pressure. It is obvious that highest temperature is equal to  $\approx 2697$  K (when  $p=170$  bar),

least – 2624 K (when  $p=110$  bar). Change of pressure within given limits is not considerably increasing the temperature of burn of the liquid fuel of such small mass as 5 mg.

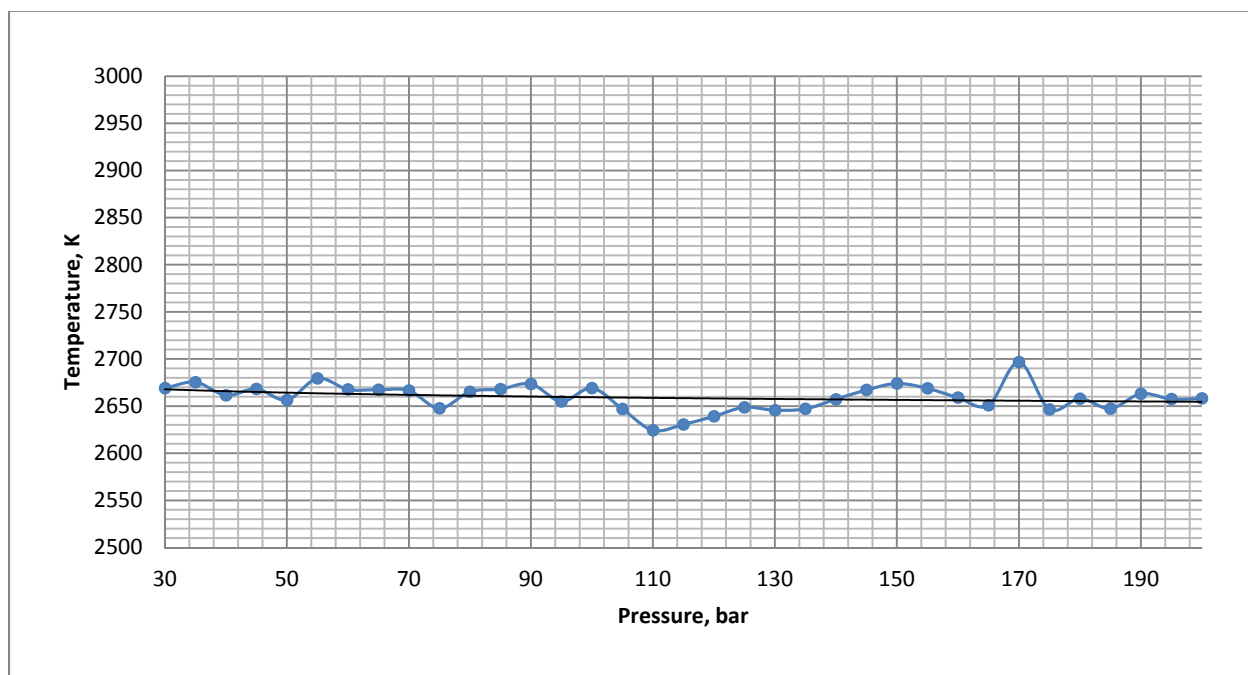


Figure 3 – Dependence of the maximum temperature from the pressure in the combustion chamber

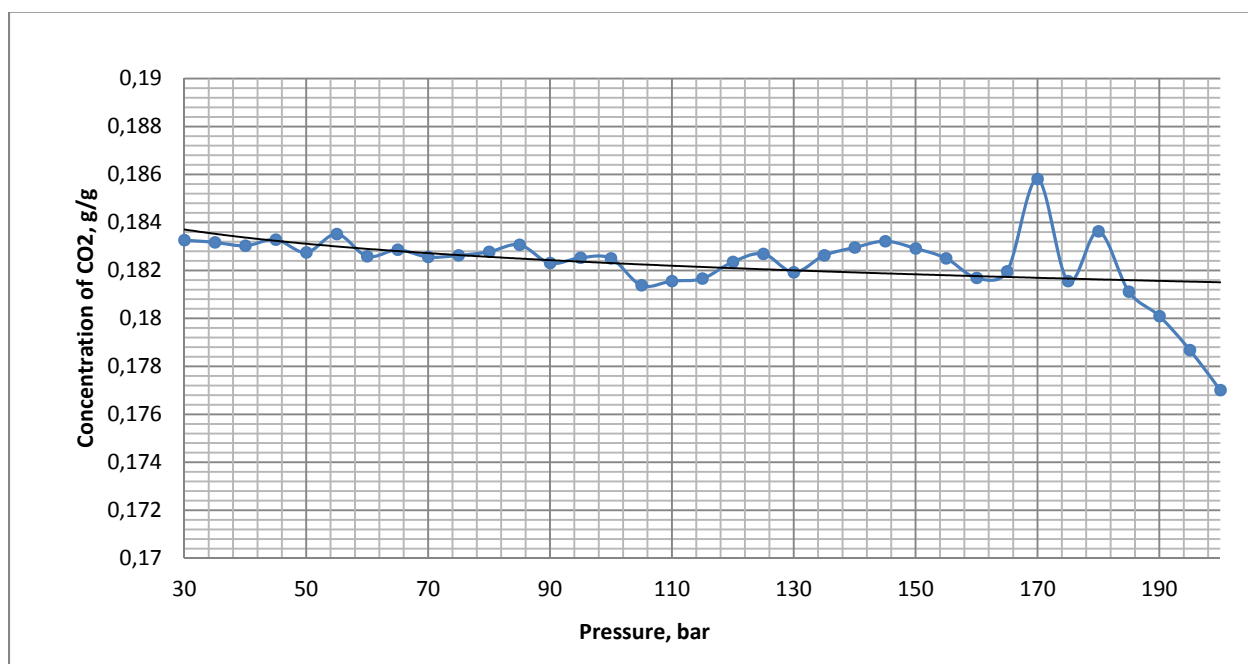


Figure 4 – Dependence of the maximum concentration of CO<sub>2</sub> from the pressure in the combustion chamber

Further given distribution of the thermal fields under  $p=170$  bar (Fig. 6). Inflammation of the fuel occurs under certain primary conditions. Further the

particles of the burning fuel, hot gases, also heat source walls of the combustion chamber are stimulating the process of heating and reaction of

burning of the newly received fuel air mixture. As you can see at the Fig.6, inflammation occurred at the period of time equal to 0.8 ms (Fig.6a), and at the period of 3.5 ms the flare reached its maximum

1.2 cm by height of the chamber and 0.5 cm by width. Core of the flame is located in the center and has temperature equal to 2697 K, and temperature at the edges of the flame is falling till 1685 K (Fig.6b).

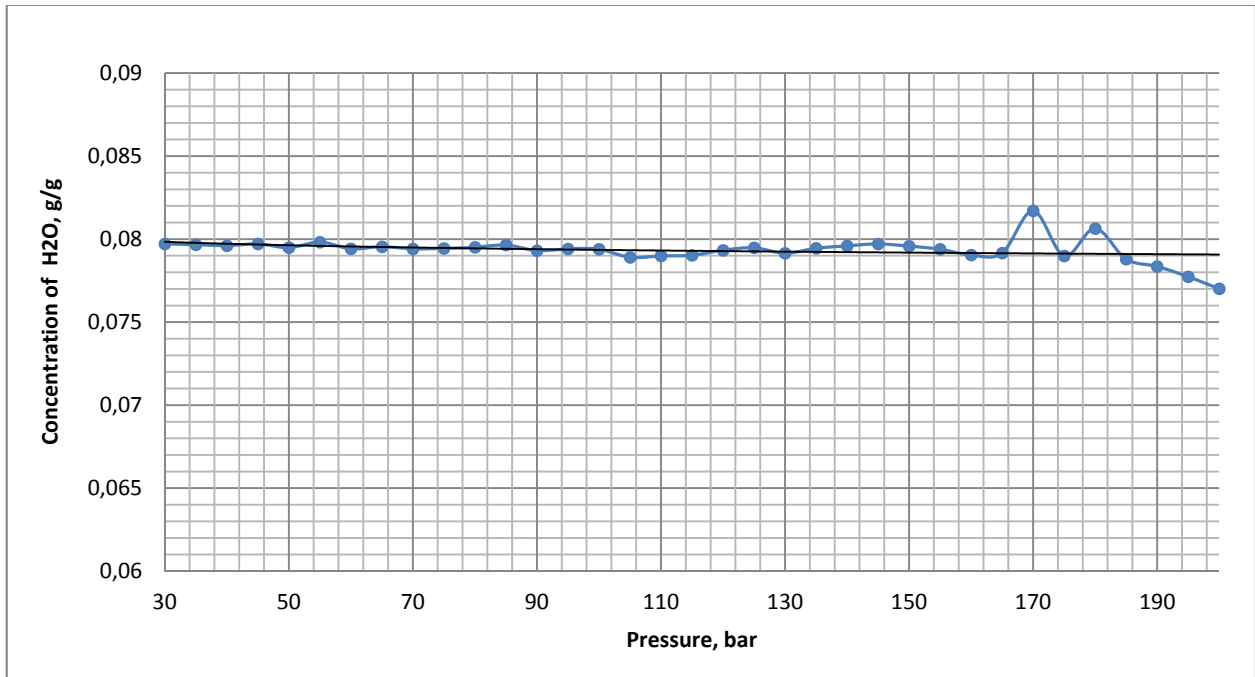


Figure 5 – Dependence of the maximum concentration of the water steam from pressure

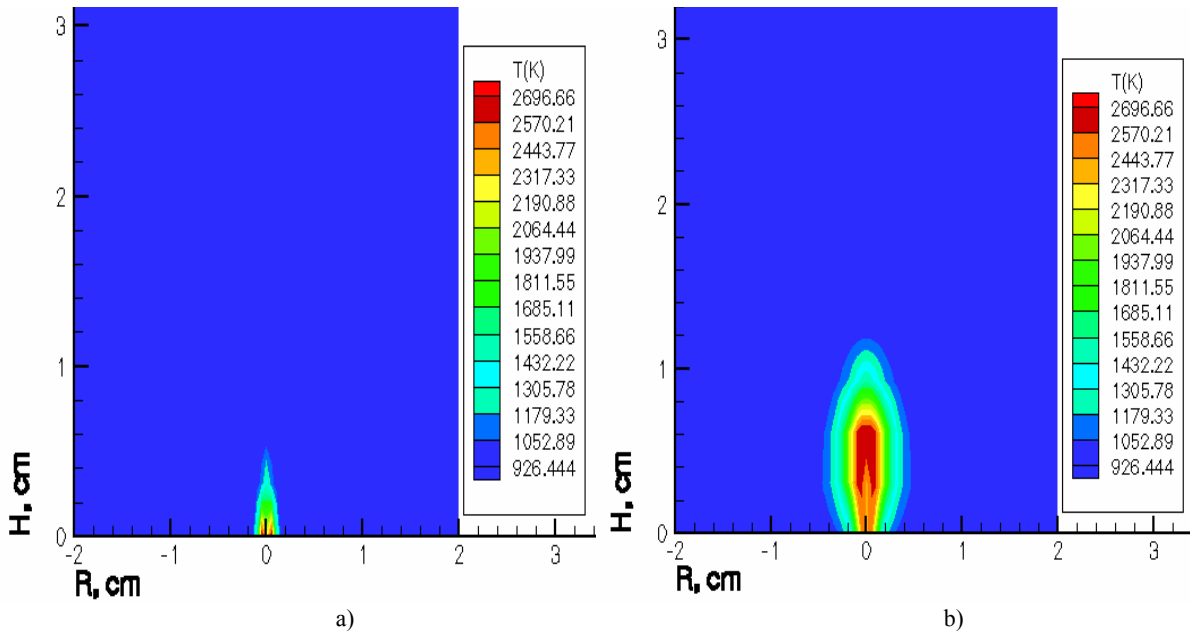


Figure 6 – Distribution of the fields (under  $p=170$  bar):  
 a) temperature at the moment of inflammation ( $t_{inflam}=0.8$  ms);  
 b) temperature at the moment of active burning ( $t=3.5$  ms).

Except emissions in to atmosphere of the 4 main air pollutants: ash, nitrogen oxide, sulfur oxide and dioxide carbon, heat and power organizations are having negative impact to the atmosphere in the result of formation of the large amount of emissions of the greenhouse gases – CO<sub>2</sub>. At the Fig.4 shown dependence of the CO<sub>2</sub> concentration from the pressure. Concentration of the carbon dioxide is reaching 0.186 g/g (under  $p=170$  bar) and is located in the maximum permissible range. Such distribution is motivated with the fact that to this value of pressure complying largest heating value of the fuel. The least concentration of the dioxide carbon is equal to 0.177 g/g (under  $p=200$  bar). Shall note that variation of the data differs only to 0.009 g/g.

At the Fig.5 shown dependence of the maximum concentration of the water steam from the pressure. At the picture shown that most concentration of H<sub>2</sub>O is equal to 0.82 g/g (under  $p=170$  bar), the least – 0.077 g/g (under  $p=200$  bar). Such distribution is repeating the data obtained at the previous Fig 5.

In the result, steady trend line of the data (Fig.2-6) is showing that depending parameters are falling with increase of pressure, we consider that the reason of it, is coalescence and decomposition of the droplets. Based on the obtained analysis, we may consider that optimal characteristics of the burning process under  $p=170$  bar, as under such pressure we notice quick inflammation of fuel 0.8 ms, maximum

heat radiation 2697 K and lower concentration of CO<sub>2</sub> 0.186 g/g. Let's review this case closely.

### Conclusion

In this work, by methods of computational modeling conducted research of the impact of pressure in the combustion chamber to the processes of inflammation and burning of hexadecane. Obtained dependence of: maximum temperature, maximum concentration of carbon dioxide, maximum concentration of the water steam, time of inflammation from pressure in the combustion chamber. Value of the pressure was increase from 30 to 200 bar (with the step of 5 bars). Obtained distribution of the temperature fields at the moment of inflammation and active combustion of fuel in the combustion chamber under optimum pressure chosen by us equal to 170 bar.

In the result of the conducted research and analysis of the results of the computational experiments, it is possible to make following conclusions:

Under the pressure equal to 170 bars noticed: 1) fast inflammation  $t_{inflamm}=0.8$  ms; 2) maximum value of heat radiation 2697 K; 3) relatively lower concentration of CO<sub>2</sub> 0.186 g/g.

Results obtained in this work will allow: 1) more efficiently combust the fuel; 2) expand the theoretic base of the physics of combustion.

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