Investigation of Various Types of Liquid Fuel Atomization and Combustion Processes at High Turbulence

Aliya Askarova, Saltanat Bolegenova, Shynar Ospanova, Symbat Bolegenova, Valery Maximov, Yrina Berezovskaya, Aizhan Nurymanova, Zhanar Shortanbayeva, Altay Tuyakbayev, Gulzhakhan Baydullayeva, Ardak Maksutkhanova, Khozyret Berdykhan, Aydana Arystan, Elmira Zulbukharova and Akmaral Sugirbekova
Al-Farabi Kazakh National University, 050040 Almaty, Kazakhstan

Abstract: This study is devoted to the study of the influence of pressure and injected mass of liquid fuels on its evaporation and combustion processes. The octane and dodecane were used as liquid fuels in the researches. There was also constructed the model of the combustion chamber in a cylinder form. During the numerical simulation an optimum combustion mode for two types of liquid fuel has been determined. Optimum pressure for octane was 100 bar and for dodecane was 80 bar. Optimal injection mass for octane was 6 mg and for dodecane was 7 mg. Numerical simulation results were compared with experimental data of various researchers. Also, for more visual description of the results of the octane and dodecane simulation processes other hydrocarbon fuels were investigated. It has been determined the amount of divergence from the simulation results of the experiment.

Key words: Atomization, combustion, turbulence, liquid fuel, internal engine, fuels

INTRODUCTION

One of complex challenges of thermal physics is the numerical study of the combustion of liquid fuels, due to accounting of a large number of complex, interrelated processes and phenomena. Therefore, numerical simulation is becoming vitally important in the area of study of combustion processes and design of different devices which use combustion process. Undoubtedly, in the future its role will increase. Having, opportunity to optimize some experiment on the basis of its virtual prototype making wide distribution of methods of computing hydrodynamics over the thermal physics. Obviously, in this days all problems arising in aerodynamics and hydrodynamics at the numerical solution of the equations of Navier-Stokes will be hardly solved. Therefore, due to the dramatic popularity of numerical studies in solving scientific and technical problems, it is necessary to ensure more possibilities of scientific and practical sides of this issue. Methods of mathematical modeling can be the most successful condition to solve practical issues in each subject area.

Improved prospects of wide using of methodology and the specific physical results in considered areas and also paths of more efficient application of methods of mathematical modeling which use the modern computer technology in various subject areas are realized by high level of researches achieved (Askarova et al., 2015a-d). It is observed that in recent years, produced 60 million cars that is approximately 165,000 cars produced per day, this is the relevance of using of liquid fuels. Now a days, car engines are significantly different from decades ago ones. The main combustion process in engines is the same but the types of injections are substantially different. For example, modern engines with electronically controlled injection system with air compression mechanism which enhances the combustion process, use only the required amount of fuel (Gorokhovski et al., 2010, 2012, 2014).

Thus, problems of saving energy and improvement of an ecological condition of heat-power object in many respects depend on the organization of high-quality combustion of fuel. However, considering that all available technologies of a fuel-preparation and combustions are practically perfect but the efficiency and ecological purity of package boilers in many cases are not well done, consequently, there is a problem of searching of new methods in the field. Simulation of the collapse, dispersion, evaporation and combustion of liquid fuel droplets under different initial conditions is relevant to solve this problems.

Introduction of new technologies requires the considerable expenses, therefore, increasing requirements

Corresponding Author: Shynar Ospanova, Al-Farabi Kazakh National University, 050040 Almaty, Kazakhstan
4054
are imposed to methods of projection and working off of equipment. Thus, now, the special attention gets not only creation of efficient physical and mathematical analogs but also development of new more perfect methods of numerical realization of systems of the subtraction equations describing a convective heat-mass transfer in combustors. Mathematical modelling of combustion of liquid fuels is the complex challenge as it requires the accounting of a large number of the complex interrelated processes and the phenomena such as multistage chain chemical reactions, transfer of an impulse, heat and weight by a convection, molecular transfer, radiation, turbulence, evaporation of drops of liquid (Askarova et al., 2014a).

Size of drops can reach several microns while the sizes of fuel channels exceed them by several times under atomization of liquid fuel by pneumatic nozzle of the gas-turbine engine. Using uniform grids in describing the collapse of the liquid film on a droplets of various sizes requires correct permission net model of phase boundaries which leads to unreasonably high computing expenses. Application of a local refinement of grids allows to manage less detailed grids and helps to approach the problem. But there is a question of influence on results of simulation of the dynamic changes of the grid model, associated with the characteristics of airborne-droplet flow instead.

**MATERIALS AND METHODS**

**Mathematical model of the problem:** The majority of currents by the nature have turbulent character, a condition of turbulence strongly influences on such parameters of a current as transfer of an impulse, temperatures and concentration of substances in the mixture during the flow motion. In this study, the thesis shows the mathematical model describing the burning of liquid fuels on the basis of the equations of conservation of mass (\( \rho \)) momentum (\( \rho \)) Energy (\( E \)) and Concentration (\( C \)):

\[
\frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{u}) = S_{\text{visc}}
\]

(1)

Where:
- \( \rho \) = The mass density of a component
- \( \mathbf{u} \) = Full mass density
- \( S_{\text{visc}} \) = The source term a local change of gas density due to evaporation or condensation

The conservation equation of an impulse of gas has the following appearance:

\[
\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \text{grad}) \mathbf{u} = \text{div} \mathbf{F} + \rho \mathbf{g} + S_{\text{visc}}
\]

(2)

\( S_{\text{visc}} = 0 \) a single-phase flow of gas

\( S_{\text{visc}} = \) The local rate of change in momentum in the gas phase due to the movement of droplets for two-phase

Conservation equation of an internal energy:

\[
\rho \frac{\partial E}{\partial t} = \mathbf{F} \cdot \mathbf{F} - \rho \text{div} \mathbf{F} - \text{div} \mathbf{S}_{\text{visc}}
\]

(3)

Where:
- \( q \) = The specific heat flux, it is the Fourier law of heat transfer
- \( \mathbf{F} \) = The rate of increase of the internal energy due to viscous dissipation source term
- \( S_{\text{visc}} \) = Denotes the contribution to the change of an internal energy due to the presence of atomized liquid or solid phase

The conservation equation of concentration of a component:

\[
\frac{\partial (\rho C)}{\partial t} + \frac{\partial (\rho \mathbf{u} C)}{\partial x} = \frac{\partial}{\partial x} \left( D - \frac{\partial C}{\partial x} \right) + S_{\text{visc}}
\]

(4)

Where:
- \( \rho \) = A mass density of a component
- \( C \) = Full mass density

More universal models in engineering calculations of turbulent flows are models with two differential equations. Using in technical flows model with two differential equation (Askarova et al., 2014d) is the most common. \( k-\epsilon \) is model when two equations for a kinetic energy of turbulence and dissipation rate are solved:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \mathbf{u} k)}{\partial x} = \frac{\partial}{\partial x} \left( \mu \frac{\partial k}{\partial x} \right) + \frac{\partial}{\partial x} \left( \frac{\mu}{\sigma_k} \frac{\partial \rho e}{\partial x} \right) - \rho \epsilon
\]

(5)

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \mathbf{u} \epsilon)}{\partial x} = \frac{\partial}{\partial x} \left( \frac{\mu}{\sigma_\epsilon} \frac{\partial \rho e}{\partial x} \right) - \epsilon
\]

(6)

This is the standard equation of \( k-\epsilon \). Values \( C_{e1}, C_{e2}, C_{\text{\epsilon}}, \sigma_k, \sigma_\epsilon \) are modal constants which are determined from the experiment. Typical values of these constants are commonly used in engineering calculations and are taken from the literature (Amsden et al., 1989, Askarova et al., 2015d).
Chemical kinetics of combustion is represented as generalized chemical reactions for the two kinds of fuel-octane and dodecane:

\[
2\text{C}_2\text{H}_4 \text{O} + 2\text{O}_2 \rightarrow 2\text{CO}_2 + 3\text{H}_2\text{O} \tag{8}
\]

\[
2\text{C}_{12}\text{H}_{26} + 37\text{O}_2 \rightarrow 24\text{CO}_2 + 26\text{H}_2\text{O} \tag{9}
\]

As a result there are the formation of the following combustion products: \text{CO}_2 and \text{H}_2\text{O}. Model of the combustion chamber in the form of a cylinder which height is 15 cm, diameter is 4 cm. The general view of the combustion chamber is shown in Fig. 1. The calculated area consists of 650 cells. Liquid fuel is injected through the nozzle which is located in the lower part of the combustor. The area of the nozzle is equal to $2\times10^{-4} \text{cm}^2$. Temperature of walls of the combustion chamber 353 K. Initial temperature of the gas in the combustion chamber 900 K, the fuel is injected at 300 K. Initial radius of injected droplets 25 \mu. The angle at which droplets are injected equal $10^\circ$. Combustion chamber pressure is 80 bar, the liquid fuel injection velocity is 250 M/s.

**Determine the optimal combustion mode:** Researches on the effect of the pressure and mass of the injection of liquid fuels on the process of atomization and dispersion of octane and dodecane in the combustion chamber are observed in this study. Also, effect of pressure on the various parameters of the combustion process of the two types of liquid fuels octane and dodecane was investigated. In the process of computing were taken experiment pressures from 20 bar with an interval of 20 bar for octane and dodecane. Similar calculations were carried out earlier by scientists of laboratory of simulation problems of a heat and mass transfer and mechanics of liquid fuel (Kazakhstan, Germany and France) which were reflected in some significant scientific works. These scientists are also search for new methods of obtaining high energy by combustion of various types of fuels. In particular, the existing practice of using expensive fuel oil or natural gas in heat energy for ignition and stabilization of low-grade coal combustion does not solve the problem as their co-firing with coal worsen major indicators of coal-fired thermal power plants (Askarova et al., 2015b, d, 2016a; Askarova et al., 2006, 2007).

Figure 2 and 3 show the temperature dependence of octane and dodecane from the pressure in the combustion chamber. By consideration of Fig. 2, it is possible to notice that the maximal temperature of drops of octane reaches 561 K with a pressure of 100 bars after which the value of temperature does not rise under the increasing of pressure of combustor chamber. For dodecane the maximal temperature 645 K corresponds to value of pressure of 80 bar and the further increase in pressure leads to decrease of temperature of drops of liquid fuel that is undoubtedly will affect deterioration of process of inflaming and further combustion (Fig. 3).
In Fig. 4, it is observed the distribution of the maximum temperature in dependence on the pressure in the combustion chamber. In comparison of curves of octane and dodecane it is seen that the maximum temperature in the combustion chamber increases during combustion of octane. The maximum temperature in the combustion chamber during combustion octane was 1948.79 K at a pressure of 100 bar. During the dodecane combustion temperature increases monotonically and reaches the highest value 1954.98 K at a pressure of 80 bar. For explanation of ranges of simulation results in case of using other fuels, we considered various researches of some researchers. In many researches, researchers investigated the dependence of the maximum combustion temperature on the fuel injection rate (Askarova et al., 2016b). By Askarova et al. (2016b) study gasoline, heptane and tetradecane are used. These fuels are often used in aviation and rocket technology. A typical configuration of air-blast atomizer in air-craft engine is shown in Fig. 5. In such injector, the liquid fuel is injected at low pressure as a thin annular liquid sheet. Two high speed airstreams co-flow along with the liquid and transfer a large amount of kinetic energy. Because of such contact with the gas-stream, the liquid sheet is sheared on either side.

This leads to disintegration of the liquid into ligaments, threads and small droplets. Figure 6 shows schematically such a type of atomization in the rocket-like conditions. Here, the central jet of liquid oxygen emerges at low velocity and is entrained into motion by high-speed stream of gaseous hydrogen. The sheared liquid jet becomes wavy with the following disruption into filaments and stripping of fine droplets by the high-speed gas motion. In both cases, it is seen that in close vicinity of injector, the liquid is not yet fragmented. Usually this zone is called as liquid core. It is defined as the area of
flow in which the fraction mass of liquid is close to unity and the liquid bulk retains as maximum unbroken (Hopfinger, 2011).

In this study, it have been conducted the influence of injection rate of liquid fuel on its combustion by numerical simulation based on the solution of differential equations of two-dimensional turbulent reacting flows. The most efficient combustion process takes place at a gasoline fuel injection speed of 200 m/sec the temperature in the chamber is set to 2330 K. For heptane and tetradecane the value of effective speed is 250 m/sec.

Temperatures in the combustion chamber are respectively 1305 and 2020 K. As can be seen from these data during the combustion of gasoline and tetradecane combustion temperature is much higher. The temperature distribution above fuel’s combustion depending on its injection speed can be seen in Fig. 7.

Also, numerical simulation results we compared with the experimental data of some researchers (Arcaumais and Gavaise, 1998). In this study, the atomization area of the liquid fuel into the combustion chamber was carried out. The researchers used a diesel, the main component of which is tetradecane. As seen in Fig. 8, the experimental points for diesel fuel (green line) and the numerical calculations for dodecane (blue line) are consistent with each other better than the numerical calculations for octane (red line).

In comparison with experiment in the initial moments of the time there is a large discrepancy with numerical calculations for both fuels. But from the time moment t - 1.5 m sec experimental data agree quite well with the results of computer simulation for dodecane. In the calculations it was determined how disagree results of numerical modeling from experimental data. For comparison we have chosen two sections from the graph. First it is the moment of t = 1 m sec where numerical modeling error was 18%. In this section simulation results are different from most of the experimental data for dodecane and diesel. In the second section (moment of time t = 2 m/sec) the number of discrepancies in the results was 0.5%. It means that in this phase points for diesel fuel best coincide with line for dodecane. Initial results discrepancy can be explained by the fact that the octane and dodecane is found in most gasoline composition, the surface tension of its is much less than that of diesel fuel.

In this study Fig. 9-10 present the results of computational experiments on changing the temporal distributions of mean Sauter diameter of Drops (SMD) of octane and dodecane with the distance from the injector. The Sauter mean diameter is the average volume-surface diameter of the drops. There is also a comparison of the results with the experimental data presented in the
Fig. 9: Comparison with the experiment of the temporal distributions of mean Sauter diameters of drops (SMD) of octane and dodecane at a distance of 40 mm from the injector.

Fig. 10: Comparison with the experiment of the temporal distributions Sauter mean diameters of drops (SMD) of octane and dodecane at a distance of 50 mm from the injector.

Fig. 11: Distribution of temperature of droplets of: a) Octane and b) Dodecane depending on the mass of the injected liquid fuel.

(Arcoumanis et al., 1998). As can be seen from the figures, the calculated and experimental data for dodecane are in good agreement. In the research (Arcoumanis et al., 1998) investigations were carried out at various distances from the injector nozzle 10, 20, 30, 40, 50 and 60 mm for dodecane. In this research a similar study was carried out at a distance from the injector nozzle x = 40 and 50 mm for the two types of liquid fuels: octane and dodecane. As can be seen from the figures, data matching and full-scale computer experiments is quite good.

Analyzing the data presented in Fig. 9-10, it can be assumed that the calculated and the experimental data are in good agreement in the case of dodecane. Analysis of the results shows good agreement of numerical results with experimental data and allows us to conclude that the proposed numerical model of the liquid fuels atomization adequately describes the actual processes of atomizing and therefore, the process of combustion of different kind of the liquid fuels.

From the analysis of the results of numerical modeling the optimum pressure for octane is 100 and 80 bar for dodecane. The temperature of drops and the combustion temperature in the combustion chamber reaches a maximum value at these pressures. At these values of pressure intensive evaporation of drops of liquid fuel begins. Also, at research of the effect of pressure in the combustion chamber on the processes of dispersion and atomization of liquid fuels it was shown that two types of fuel pressure rise leads to increase in area of high temperatures (Askarova et al., 2013, 2014c).

There are the computer experiments on the effect of injection mass of liquid fuels (octane and dodecane) into the combustion chamber in the combustion process were made in this experiment. These calculations were carried out at the optimal values of the combustion chamber pressure 100 bar for octane and 80 bar for dodecane. At calculations the mass of fuel varied from 4-20 mg.

Figure 11-12 show the results of computational experiments on the effect of the mass injection of liquid fuels on the combustion process of octane and dodecane. Figure 11 shows the temperature distribution of octane and dodecane droplets on volume of the combustion chamber depending on the mass of injection of liquid fuel.

Analysis of Fig. 11a shows that, the increase of the mass of injection leads to temperature increase for octane and at 6 mg, its value amounted to 562 K. Figure 11b shows a similar distribution of dodecane droplets at
Fig. 12: Distribution of concentration of carbon dioxide during the octane's (red line) and dodecane's (blue line) combustion in the combustion chamber depending on the injection mass of liquid fuel

various values of the injection mass. The maximum temperature for dodecane 644 K, occurs at a mass of 7 mg as shown in Fig. 11 and 12 show the effect of the mass injection of octane and dodecane on the distribution of the concentration of carbon dioxide. Analysis of the curves shows the increase of concentration of CO₂ with increasing of injection mass of liquid fuel. At the injection mass equal 6 mg for octane and 7 mg for dodecane a small concentration of carbon dioxide within the permissible limits is allocated (Askarova et al., 2014b).

Overall, it can be concluded that optimal octane mass for injection is 6 and 7 mg for dodecane. At this values of the injection mass of liquid fuel temperature reaches the maximum value. Further increase of the injection mass for both octane and dodecane at optimal pressures make worth the combustion process and leads to a further lowering of the temperature (Askarova et al., 2012a, b, 2007).

RESULTS AND DISCUSSION

Figures 13 and 14 show the results of numerical simulation of combustion of octane and dodecane in the combustion chamber at the optimal pressure and mass values. Figure 13 shows the distribution of octane droplet by sizes by height of chamber at time t = 2.5 msec. At time t = 2.5 msec octane and dodecane droplets rose to the camera height equal to 0.62 and 0.72 cm, respectively. Analyzing the behavior of dodecane it is noticed that it drops rise to a height of 0.72 cm at time t = 2.5 m sec and the droplets sizes slightly larger droplets of octane (Fig. 13b).

Paying attention to distribution of octane and dodecane on radiuses it is possible to notice that dodecane droplets evaporate quickly and the distribution density is higher. Also, the size of droplets of octane grows by time. Thus, for example, at the time of 2 msec in the lower part of the chamber located droplets with a radius of 0.021762 mm. And at this time dodecane droplets with the same sizes completely burned out and droplets with smaller radiuses move up by chamber height to an exit.

Figure 14 shows the temperature field in the combustion chamber during combustion of octane and dodecane at time t = 2.5 msec. These charts indicates that during the combustion of octane the large part of chamber warmed to 987.192 K, during the dodecane combustion chamber held longest value of the temperature equal to 1003.05 K. At time t = 2.5 msec in the core of temperature flame temperature reaches a value of 2687.32 K during the combustion of octane (Fig. 14a).

During the combustion of dodecane maximum temperature was 2679.87 K and the temperature of the chamber, except for the zone of plumes reaches 1003.05 K (Fig. 14b). There is following situation for the temperature distribution of two types of fuels: the area covered by the maximum temperature during combustion of both fuels at different points of time almost the same. But during combustion of dodecane temperature of whole volume of chamber hatred faster in comparison with octane. Analyzing the data obtained, we can conclude that the process of combustion of octane and dodecane occurs in the gas phase and over the whole volume of the combustion chamber there is a uniform temperature distribution.

Figure 15 shows field concentration both fuels at different times of combustion. It is observed in the figures, that the pair of octane and dodecane at time t = 2.5 msec have a certain concentration. So, for the octane value of the concentration was 0.04739794 g/g and for dodecane 0.3603 g/g. In comparison the octane and dodecane it is shown that a pair of both fuels rise to different heights. For example, at time t = 2.5 msec pair octane climb chamber height of 2.3 msec and a pair of dodecane at the same time located at a height of 2.6 cm.

Figure 16 shows for comparison the combustion temperature distributions of gasoline, heptane and tetradecane at optimum combustion mode. Analysis of Fig. 16 shows the change in temperature in the combustion chamber for the three kinds of fuels. It can be seen that the area of maximum temperature of gasoline
Fig. 13: Distribution of droplets of octane and dodecane by radius by height of combustion chamber at time $t = 2.5$ m sec: a) Octane and b) Dodecane.

Fig. 14: Temperature profiles in the combustion chamber during the combustion of octane and of dodecane at time $t = 2.5$ msec: a) Octane and b) Dodecane.

The core of the torch reaches 6.5 cm in height of the combustion chamber, the rest of the chamber is heated to 1300 K (Fig. 16a).

Results for heptane and tetradecane similar to results for gasoline in qualitative terms, differing quantitatively. Analysis of Fig. 16b shows that the maximum temperature in the combustion chamber during combustion of heptane equal to 1300 K at time 4 msec. The remainder of the chamber maintains the initial temperature of 900 K. Analysis of Fig. 16c shows that the greatest value which warms up combustion chamber by burning tetradecane, temperature is equal to 2022 K where in the torch is a temperature higher than that of heptane (Fig. 16b). The chamber temperature at the final time 4 m sec sis 1200 K.
Fig. 15: Distribution octane and dodecane vapor by height of combustion chamber at time t = 2.5 msec: a) Octane and b) Dodecane

Fig. 16: The temperature distribution in the combustion chamber during the combustion of various kinds of liquid fuel at time of 4 msec: a) Gasoline; b) Heptane and c) Tetradecane

CONCLUSION

This study is devoted to the influence of various parameters on the processes of combustion of hydrocarbon liquid fuels. During the research two kind of liquid fuels were used octane and dodecane which are often used as a technical fuel in the aviation technical equipment and passenger cars. During the study the influence of the initial gas pressure in the combustion chamber on the combustion processes was investigated. Analysis of the numerical simulation results leads to the conclusion that the best for octane is a pressure of 100 bar and 80 bar dodecane. At these pressures, the temperature of the drops and the combustion temperature in the combustion chamber reaches the maximum values. Under these pressures intensive evaporation of the liquid fuel drops begin. Also, in the study of the influence of pressure in the combustion chamber on the processes of the atomization and dispersion of liquid fuel has been shown that for the two fuels increase in pressure causes an increase high temperatures.

Also, in the research were conducted computer experiments on the influence of the injection mass of the liquid fuel (octane and dodecane) into the combustion chamber on the combustion process. As a result of numerical investigations we can conclude that the optimal
injection mass for octane is 6 mg and for dodecane is 7 mg. For these values of the injection mass of the liquid fuel the temperature reaches the maximum value. A further increase in the mass of injection for octane and dodecane for at optimum pressures worsen the combustion process and leads to a further reduction of temperature.

Also, the results of numerical simulations were compared with experimental data, obtained by various authors. Atomization areas of the liquid fuel and the temporal distributions of the mean Sauter diameter of the drops at different distances from the injector were obtained. The results of numerical simulation in this case was given a good agreement with experiment. Also, for comparison of characteristics of various liquid fuels combustion processes has been studied three types of fuels. Verification of obtained during the computational results of the experiments, a comparison with experimental data and theoretical calculations have revealed good agreement.

IMPLEMENTATIONS

The scientific importance the research is that the results obtained in this research can be applied in the construction of liquid fuel combustion theory and will contribute to a better understanding of the complex physical and chemical phenomena that occur in the combustion chambers. The practical significance of the conducted computational experiments in the research is that the results can be used in the design of a variety of internal combustion engines which would simultaneously solve the problem of optimizing the combustion process, increase fuel efficiency and minimize emissions. The results are implemented in the educational process in the form of textbooks, manuals and virtual computer laboratory works on physics of combustion and numerical methods of thermal physics which reflect modern approaches to organizing a special workshop intended for students in higher educational establishments specializing in the field of technical physics, thermal energy and computational fluid dynamics.

REFERENCES


