Maciej SIDOROWICZ Ireneusz PIELECHA CE-2017-309

Inflammability evaluation of hydrocarbon fuels mixtures formed directly in the combustion chamber

The proposed article involves an investigation of the processes taking place during the preparation of mixed fuels that are combined directly before combustion. The fuel dose formed in this way must take into account the qualitative and quantitative composition of the fuels and the amount of air in the process. Given that liquid fuels similar to gasoline (e.g. methanol, ethanol, butanol) are characterized by different properties, their comparison would be useful in order to use their ratio to influence the combustion process. The process of fuel preparation plays a decisive role in this issue.

The article describes abilities of modelling the injection of various fuels simultaneously to the combustion chamber for creating fuel mixture directly before ignition. First part of the article consists of analysis of light hydrocarbon fuels mixing abilities, supported with present research data. Next part describes the evaluation of execution of the assumed system – two fuel injectors with analysis of spray penetration. The modelling of the injection and spray was performed in the AVL FIRE 2014.2 environment and the results were presented. The injection possibility was proven by injecting the fuel to the combustion chamber model. Local values of air-fuel ratio, density and ambient pressure were presented to better understand the potential in mixing fuels directly before ignition. The conclusion includes description of fuel mixing abilities, influence of various fuels on creation of a stratified mixture and definition of controllability of charge ignition.

Key words: fuel injection, mixing fuels, hydrocarbon fuels, combustion chamber

1. Introduction

Combustion processes are considered mainly in terms of a mono-fuelled combustion. Processes of preparation and combustion of gasoline-like fuels are widely described in literature.

Dual-fuel mixtures are crated mostly in the earlier process (for example, a mixture of ethanol and gasoline or petrol and methanol [12, 17]) and are burned most often in stoichiometric conditions. The way of preparing such a mixture causes it to have specific physico-chemical properties (viscosity, surface tension and density closely define specific contents of different hydrocarbon groups) [12, 22]. In such a situation, sprays of drops with small, homogeneous dimensions are obtained. Figure 1 shows a typical process of fuel flow from the injector [2].

The air with high temperature is "incorporated" into the fuel spray. The hot air causes fuel evaporation, and as a result the length of the spray is reduced. After the initiation of combustion, a slight reduction of the spray takes place and then its length stabilizes before the end of the injection. The diffusion flame is formed in the areas where the mixture reaches a value close to stoichiometric. The rich flammable mixture zone is an area in which the formation of particulate matter is initiated. This results in a significant concentration of soot in the diffusion flame of the burned fuel. The pre-flame zone (outer) is "responsible" for the formation of nitrogen oxides [3].

Gasoline is a mixture of over 100 different hydrocarbons having different molecular structure and different boiling points. Most often the structure of gasoline consists of about 55% paraffins (single-bond C–C), around 35% aromatic hydrocarbons (benzene rings) and a maximum of up to 20% olefins (double bond C=C). Paraffins are complex components with low molar mass: these are e.g. nbutane, 2-methyl-pentane and 2,2,4-trimetyl-pentane (isooctane). Aromatic hydrocarbons contain 4 to 8% toluene and around 4% xylene.

The oxidizing additives used in gasoline increase its octane number. The influence of additives on the octane number is dependent on the fuel composition. Gasoline is enriched with alcohols (R-O-H, where R is the HC group) and ethers (R-O-R). Alcohols are mainly methanol (MeOH), ethanol (EtOH), isopropanol (IPA) and t-butanol (TBA). Due to the weak solubility of methanol in gasoline in the presence of water, it must be used together with TBA as a co-solvent. Ethers used as additives include mainly: methyl tert-butyl ether (MTBE), tert-amyl methyl ether (TAME) and ethyl tert-butyl ether (ETBE).

Use of previously proposed fuels to determine the properties of the mixtures, requires knowledge of their physicochemical properties. Physical properties of such fuels should play an important role in the mixing processes.

The distillation curve of gasoline, taking into account that gasoline is a mixture of different hydrocarbons, is shown against the background of basic fuels (Fig. 1).



Fig. 1. Distillation curve of gasoline and other fuels [1]

Also the physico-chemical properties of all the analysed fuels are known. Although o-xylene, presented in Figure 2, has a boiling point close to the last value of boiling point for gasoline, it was also qualified in the study as a standalone fuel submitted to mixing. The coefficients for determining fuel vapour pressure were presented e.g. by [7] and they can be used in the equation [1]:

$$\ln(p_i) = A - B/(T_i + C)$$
(1)

where A, B, and C are Antoine constants for pure components (e.g. water, methanol or ethanol) obtained from literature data.



Fig. 2. Fuel vapours pressure

The exchange of mass between the surface of the fuel drop and the gaseous medium (air) occurs due to molecular and turbulent diffusion. The molecular diffusion is the spontaneous mixing of fuel and air particles as a result of concentration gradient dc/dr, which excites the flow of heat and, induced by this, the flow of mass (thermo-diffusion). In case of creating a flammable mixture diffusion caused by a gradient of concentration of components is of crucial significance. Molecular diffusion, characterised by diffusion coefficient (D_M) , is of vital importance in case of the lack of flow or laminar flow. In this case, mixing of the components is caused by random movement of their particles. In case of turbulent flow, the mass exchange is more intense due to the movements of particles in normal direction. The turbulent diffusion coefficient (D_T) has much higher value than the D_M coefficient. During the diffusion of vapour from the surface of the drop of fuel, surrounded by turbulent air jet, the surface layer δ consists of the first sub-layer, contacting the surface of the liquid, and the second layer located on the outside of the first. In the first sublayer a molecular diffusion takes place, and on the other layer - it's mainly turbulent diffusion.

Many publications [e.g. 1, 20] claim that penetration of sprays chosen for testing fuels shows a similar linear scope. This indicates similar physical properties of these fuels. At the same time, it should be noted that such similarity is a positive feature, as it can alter the properties of ignition of mixtures without a significant change in parameters of their atomisation. These changes are visible only during significant heating of fuels (above 373 K). Then the penetration of pentane and ethanol is lower by about 10% [1].

The effect of flow turbulence can be characterized by the Reynolds number (Fig. 3):

$$\operatorname{Re} = \rho \cdot u \cdot d/\mu \tag{2}$$

where ρ – is density, μ – kinematic viscosity of liquids, d – diameter of the injector aperture, u – flow rate.

The lowest Reynolds number (at constant flow parameters) can be observed for butanol (laminar flow at low temperatures of the fuel).



Fig. 3. Reynolds number of selected fuels [1]

The fuels selected for analysis are characterized by a Weber number above 50. With the increasing temperature, this value also increases: for o-xylene it is 120 and for the remaining fuels much more (for iso-octane -230) at a temperature of about 453 K. These figures result from the specificity of the adopted characteristic values, requiring calculation of We number [1].

In publication [15] it was shown that the Weber numbers for ethanol and gasoline are similar for fuel temperatures ranging from 275-450 K. Further increase of the temperature causes an increase of Weber number for ethanol above 500 (in temperature of 500 K), while for petrol it is about 300 (temperature 500 K). This means that at high temperatures of the fuel the so-called catastrophic breakdown of ethanol drops occurs.

Ohnesorge number is convergent with the data contained in the publications [4, 8] and amounts to about $6 \cdot 10^{-3}$ to $1.6 \cdot 10^{-2}$ at the temperature of about 283 K, and decreases to a value of about $6 \cdot 10^{-3}$ for temperature of 463 K.

Indication of these differences is a basis for the conclusion that the created drops of fuel will also have different diameters, which will contribute to their diversified evaporation.

Combustion in dual-fuel systems of fuel mixtures created immediately before ignition makes it possible to determine the combustion air factor, which will be the resultant of the ratio of both fuels:

$$\lambda = \frac{m_{air}}{L_1 m_1 + L_2 m_2} \tag{3}$$

where: L_1 and L_2 are stoichiometric air requirements for combustion of fuel 1 and 2, m – is weight of fuel, respectively 1 and 2, m_{air} – is the weight of air. The share of one of the fuels can be calculated from the following:

$$U_{m2} = \frac{W_{op_2}m_2}{W_{op_1}m_1 + W_{op_2}m_2}$$
(4)

Determination of inhomogeneity of the mixtures created immediately before combustion leads to the assessment of production of soot originating from the inhomogeneity of the charge in the process of mixing the air-fuel charge. The global index of uniformity is referred to as [18]:

$$U_{I} = 1 - \sigma/\sigma_{\nu,\eta} \tag{5}$$

where σ determines the standard deviation of the fuel mass distribution, and $\sigma_{n,h}$ is defined as the standard deviation of the completely inhomogeneous charge (fuel and air):

$$\sigma_{n,h} = \frac{\sqrt{A/F}}{1 + A/F} \tag{6}$$

However, the U_1 parameter is not fully representative of the possibility of determining the distribution of fuel vapour with division into rich and lean zones. Also the analysis associated with post-processing of the images from such a process is required. This index takes the maximum value equal to 1 for completely homogeneous mixtures. It is a good indicator of mixing fuels proposed for tests in the current research.

2. Motivation

The process of combustion of liquid fuels (gasoline, ethanol, methanol, n-butanol and its mixtures) is characterized by high variability of the thermodynamic conditions. The process of combustion of liquid fuels may be continuous or cyclical. In the first case there are stabilized thermodynamic conditions, and in the other case – the conditions are changing. Due to significant changes in combustion conditions (temperature, pressure), the process of preparing the mixture is short, which is one of the main causes of its unrepeatability. In such a short time the initial physical processes of mixing fuel with air and the pre-flame processes take place (chemical evaporation of fuel and its thermal decomposition). During this period the reactions and processes leading to formation of toxic components also begin take place. Some scientists assume [27] that oxidation and products of thermal decomposition of the liquid fuel molecules can be important intermediate stages in the formation of particulate matter.

The dominant trend concerning combustion of liquid fuels is delivering them in the form of previously created mixtures: e.g. gasoline-ethanol or gasoline-methanol in various proportions. It is justified from chemical perspective to create mixtures with very specific proportions in order to ensure the homogeneity of such a mixture.

However, there are no descriptions in the literature of possibilities of creating mixtures of fuels directly before their combustion in open or closed chambers. Knowing that liquid hydrocarbon fuels (similar to gasoline) have different properties, it is reasonable to mix them in such a way that the proportions can influence the combustion process. Currently this is not possible, because the composition of fuels (proportions) is strictly defined prior to combustion. Different parameters of volatility, vapour pressure or octane number can provide a method of controlling the process of their combustion in a wide range. However, before such combustion can take place, it is necessary to recognize both the physical and chemical processes of mixing such fuels immediately before ignition.

3. Research methodology

The research was performed by means of computer aided simulation using the AVL Fire 2014.2 software environment.

The combustion chamber used in the research was modeled to comply with the assumed engine parameters, listed in the Table 1.

Table	1	Modeled	engine	technical	data
1 able	1.	woucieu	engine	technical	uala

		8
Parameter	Unit	Value
Туре	1	Piston engine, 4-stroke, spark ignition
Cylinder number	-	1
Displacement	cm ³	385
Compression ratio	-	10.2
Bore	mm	83
Stroke	mm	71.2

The research consisted of performing the direct fuel injection events into the modeled combustion chamber through two separate injectors. The indicative view of the injectors positioning in the combustion chamber is presented in Fig. 4.

Three combinations of fuels injected with separate injectors were used:

- gasoline from both injectors,
- gasoline and methanol,
- gasoline and iso-pentane.

The injectors were oriented so their axes formed a 45° angle with the cylinder axis. Each simulation included single injections of constant mass of fuel. The injections were open for a constant amount of time (CA-wise) and were initiated with the same timing. The injectors' and spray parameters are listed in Table 2.

Table 2. The parameters of injectors and spray

Parameter	Unit	Value
Injectors type	-	Outward opening
Nozzle apex angle	deg	95
Spray angle	deg	10
Nozzle outer diameter	mm	2
Nozzle inner diameter	mm	1.5
Spray type	-	hollow cone
Injection beginning	deg CA	35 before TDC
Injection end	deg CA	25 before TDC
Injected mass per event	mg	30
Drag law model	-	Schiller-Naumann
Fuel evaporation model	-	Dukowicz ('Gasoline')
		Multi-component (others)
Fuel breakup model	-	Wave

The Schiller-Naumann drag law model Cd is an empirically evaluated equation for calculating drag coefficient in drag force acting on the flowing particles in fluid with Re ranging from 0.2 to 1000. It is described with the equation:

$$Cd = \frac{^{24}}{^{Re}}(1 + 0.15Re^{0.687})$$
(7)

where Re is the Reynolds number. For the Re > 1000 the Cd has the constant value of 0.44 [5].

The Dukowicz evaporation model describes the heat and mass transfer processes on the droplet-fluid border. The model is based on the following assumptions:

- spherical symmetry,

- quasi steady gas-film around the droplet,

- uniform droplet temperature along the drop diameter,
- uniform physical properties of the surrounding fluid,
- liquid-vapor thermal equilibrium on the droplet surface.

The vapor mass flux $(\dot{q_s})$ to local surface heat flux $(\dot{q_s})$ ratio is, according to the Dukowicz model, calculated as per formula (8):

$$\frac{\dot{f_{vs}}}{\dot{q_s}} = \frac{-B_y}{h_{\infty} - h_s - (h_{vs} - h_{gs})(Y_{v\infty} - Y_{vs})}$$
(8)

where B_y is mass transfer number, h_∞ is enthalpy in particle far-field condition, h_s is enthalpy at particle surface, h_{vs} is enthalpy in vapor conditions at droplet surface, h_{gs} is enthalpy in ambient gas conditions at droplet surface, $Y_{v\infty}$ is vapor mass fraction in particle far-field condition, Y_{vs} is mass fraction in vapor conditions at droplet surface [5].

The Multi-component evaporation model is the extension of the Abramzon-Sirignano approach. The difference to single-component cases is that the mass transfer of every component is taken into account separately, whereas the heat transfer remains a global mechanism. The resulting mass flow rate then is the sum of the single contributions:

$$\dot{\mathbf{m}} = \sum_{i=1}^{N} \dot{\mathbf{m}}_i \tag{9}$$

The distribution of the components inside the droplet is assumed to be homogeneous [5]. This model is required to be used in multi-fuel spray calculations.

The Wave breakup model describes the spray into droplet breakup behaviour. Initial spray assumption is that the blob injection is realized (initial droplet size is similar to the nozzle diameter). The quasi-continuous fuel stream is broken up to droplets as per Wave model. It assumes that the growth of an initial perturbation on a liquid surface is linked to its wavelength and toother physical and dynamic parameters of the injected fuel and the domain fluid. For the high pressure injection systems (high spray velocity) the size of the product (parent) droplets is set equal to the wavelength of the fastest growing or most probable unstable surface wave. For lower velocities, the Rayleigh type breakup is applied [5].



Fig. 4. The indicative view of positioning the direct injection fuel injectors

The model engine data are presented in Table 1, whereas the combustion chamber view with positioned injectors in it in Fig. 4. The visible two injectors are mounted instead of valves. Such configuration of the fuel injection into the area of centrally positioned spark plug (Fig. 5) allows the execution of spray-guided type mixture creation.



Fig. 5. The part-section view of the combustion chamber with outlined spark plug in the centre of the chamber

In the AVL Fire 2014.2 software using the Fame Engine+ module the displaceable mesh was created (Fig. 6), in which the following selections were assigned:

- piston buffer,
- piston moving
- piston non_moving.

The created mesh of size of 211 thousand cells (Table 3) served as the model for injection and spray analysis of various fuels.



Fig. 6. The displaceable mesh of combustion volume for fuel spray simulation

Table 3. The computational mesh parameters

Mesh info	Value
Number of nodes	203732
Number of surface faces	40240
Number of tet cells	2200
Number of hex cells	160022
Number of pyramid cells	15908
Total number of cells	211406
Surface area	0.027 m^2
Volume	0.0003362 m ³

4. The fuels' injection and spray processes analysis

The presented simulations concerning fuels' spray cover the injection analysis of gasoline, ethanol and iso-pentane in various configurations of their delivery to the combustion chamber. Varied properties of these fuels, presented in point 2 and Table 4, point at possibilities of air excess ratio shaping in combustion chamber during their direct mixing before ignition.

$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Parameter	Unit		Fuel	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			Gasoline	Ethanol	Iso-pentane
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Chemical formu-	-	C ₈ H ₁₅	C ₂ H ₅ OH	C5H12
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	la				
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Composition	%	86,14,0	52,13,35	87,13,0
Research octane number-95 [29]106 [14]100 [21]Density@ 20°Ckg/m³744.6 [29]790.9 [29]616 [28]Lower heating valueMJ/kg43.5 [11]27.0 [11]44.91 [10]Viscosity @25°Cmm²/s0.4-1 [16]1.32 [19]0.35 [23]Dynamic viscos- ity @ 25°CmPa s5.29 [26]1.104 [25]0.22Surface tensionN/m0.022 [9]0.02230.016[6]Enthalpy of evaporationkJ/kg373 [29]840 [29]342 [23]Stoichiometric A/F ratio-14.6 [11]9.0 [11]38.1 [6]Saturation edg CkPa31 [11]13.8 [11]128 [13]Flash point°C-45 to-38 [11]21.1 [11]-50 [23]Auto-ignition temp.°C32.8 [29]78.4 [29]27.9 [28]	(C,H,O)				
number \sim \sim Density@ 20°C kg/m ³ 744.6 [29] 790.9 [29] 616 [28] Lower heating value MJ/kg 43.5 [11] 27.0 [11] 44.91 [10] Viscosity mm ² /s 0.4–1 [16] 1.32 [19] 0.35 [23] @25°C mPa s 5.29 [26] 1.104 [25] 0.22 Dynamic viscos- ity @ 25°C mPa s 5.29 [26] 1.104 [25] 0.22 Surface tension N/m 0.022 [9] 0.0223 0.016[6] Enthalpy of evaporation kJ/kg 373 [29] 840 [29] 342 [23] Stoichiometric A/F ratio - 14.6 [11] 9.0 [11] 38.1 [6] Saturation kPa 31 [11] 13.8 [11] 128 [13] pressure at 38 deg C - - -50 [23] Flash point °C -45 to-38 [11] 21.1 [11] -50 [23] Muto-ignition °C 32.8 [29] 78.4 [29] 27.9 [28]	Research octane	-	95 [29]	106 [14]	100 [21]
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	number				
Lower heating valueMJ/kg $43.5 [11]$ $27.0 [11]$ $44.91 [10]$ Viscosity @25°Cmm²/s $0.4-1 [16]$ $1.32 [19]$ $0.35 [23]$ Dynamic viscos- ity @ 25°CmPa s $5.29 [26]$ $1.104 [25]$ 0.22 Surface tensionN/m $0.022 [9]$ 0.0223 $0.016[6]$ Enthalpy of evaporationkJ/kg $373 [29]$ $840 [29]$ $342 [23]$ Stoichiometric A/F ratio- $14.6 [11]$ $9.0 [11]$ $38.1 [6]$ Saturation gressure at 38 deg CkPa $31 [11]$ $13.8 [11]$ $128 [13]$ Flash point°C $-45 to-38$ $21.1 [11]$ $-50 [23]$ Auto-ignition temp.°C $32.8 [29]$ $78.4 [29]$ $27.9 [28]$	Density@ 20°C	kg/m ³	744.6 [29]	790.9 [29]	616 [28]
value mm²/s 0.4–1 [16] 1.32 [19] 0.35 [23] @25°C mPa s 5.29 [26] 1.104 [25] 0.22 Dynamic viscos- ity @ 25°C mPa s 5.29 [26] 1.104 [25] 0.22 Surface tension N/m 0.022 [9] 0.0223 0.016[6] Enthalpy of evaporation kJ/kg 373 [29] 840 [29] 342 [23] Stoichiometric A/F ratio - 14.6 [11] 9.0 [11] 38.1 [6] Saturation kPa 31 [11] 13.8 [11] 128 [13] pressure at 38 deg C - -45 to-38 21.1 [11] -50 [23] Flash point °C 420 [11] 434 [11] 468 [23] temp. - 32.8 [29] 78.4 [29] 27.9 [28]	Lower heating	MJ/kg	43.5 [11]	27.0 [11]	44.91 [10]
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	value				
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Viscosity	mm ² /s	0.4-1 [16]	1.32 [19]	0.35 [23]
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	@25°C				
ity @ 25°C 0 0 0.022 [9] 0.0223 [25] 0.016[6] Surface tension N/m 0.022 [9] 0.0223 [25] 0.016[6] Enthalpy of evaporation kJ/kg 373 [29] 840 [29] 342 [23] Stoichiometric A/F ratio - 14.6 [11] 9.0 [11] 38.1 [6] A/F ratio kPa 31 [11] 13.8 [11] 128 [13] pressure at 38 deg C - - - - Flash point °C -45 to-38 21.1 [11] -50 [23] Auto-ignition temp. °C 32.8 [29] 78.4 [29] 27.9 [28]	Dynamic viscos-	mPa s	5.29 [26]	1.104 [25]	0.22
Surface tension N/m 0.022 [9] 0.0223 [25] 0.016[6] Enthalpy of evaporation kJ/kg 373 [29] 840 [29] 342 [23] Stoichiometric A/F ratio - 14.6 [11] 9.0 [11] 38.1 [6] Saturation kPa 31 [11] 13.8 [11] 128 [13] pressure at 38 deg C - -45 to-38 21.1 [11] -50 [23] Flash point °C -45 to-38 21.1 [11] -50 [23] Muto-ignition temp. °C 32.8 [29] 78.4 [29] 27.9 [28]	ity @ 25°C				
Enthalpy of evaporation kJ/kg 373 [29] 840 [29] 342 [23] Stoichiometric A/F ratio - 14.6 [11] 9.0 [11] 38.1 [6] Saturation kPa 31 [11] 13.8 [11] 128 [13] pressure at 38 deg C - -45 to-38 21.1 [11] -50 [23] Flash point °C -45 to-38 21.1 [11] -50 [23] Auto-ignition temp. °C 32.8 [29] 78.4 [29] 27.9 [28]	Surface tension	N/m	0.022 [9]	0.0223	0.016[6]
Enthalpy of evaporation kJ/kg 373 [29] 840 [29] 342 [23] Stoichiometric A/F ratio - 14.6 [11] 9.0 [11] 38.1 [6] Saturation kPa 31 [11] 13.8 [11] 128 [13] pressure at 38 deg C - -45 to-38 21.1 [11] -50 [23] Flash point °C -45 to-38 21.1 [11] -50 [23] Muto-ignition temp. °C 32.8 [29] 78.4 [29] 27.9 [28]				[25]	
evaporation - 14.6 [11] 9.0 [11] 38.1 [6] Stoichiometric A/F ratio - 14.6 [11] 9.0 [11] 38.1 [6] Saturation pressure at 38 deg C kPa 31 [11] 13.8 [11] 128 [13] Flash point °C -45 to-38 [11] 21.1 [11] -50 [23] Auto-ignition temp. °C 420 [11] 434 [11] 468 [23] Boiling point °C 32.8 [29] 78.4 [29] 27.9 [28]	Enthalpy of	kJ/kg	373 [29]	840 [29]	342 [23]
Stoichiometric A/F ratio - 14.6 [11] 9.0 [11] 38.1 [6] Saturation pressure at 38 deg C kPa 31 [11] 13.8 [11] 128 [13] Flash point °C -45 to-38 [11] 21.1 [11] -50 [23] Auto-ignition temp. °C 420 [11] 434 [11] 468 [23] Boiling point °C 32.8 [29] 78.4 [29] 27.9 [28]	evaporation				
A/F ratio kPa 31 [11] 13.8 [11] 128 [13] Saturation pressure at 38 deg C -45 to-38 [11] 13.8 [11] -50 [23] Flash point °C -45 to-38 [11] 21.1 [11] -50 [23] Auto-ignition temp. °C 420 [11] 434 [11] 468 [23] Boiling point °C 32.8 [29] 78.4 [29] 27.9 [28]	Stoichiometric	-	14.6 [11]	9.0 [11]	38.1 [6]
Saturation pressure at 38 deg C kPa 31 [11] 13.8 [11] 128 [13] Flash point °C -45 to-38 [11] 21.1 [11] -50 [23] Auto-ignition temp. °C 420 [11] 434 [11] 468 [23] Boiling point °C 32.8 [29] 78.4 [29] 27.9 [28]	A/F ratio				
pressure at 38 deg C °C -45 to-38 [11] 21.1 [11] -50 [23] Flash point °C 420 [11] 434 [11] 468 [23] Auto-ignition temp. °C 32.8 [29] 78.4 [29] 27.9 [28]	Saturation	kPa	31 [11]	13.8 [11]	128 [13]
deg C °C -45 to-38 21.1 [11] -50 [23] Flash point °C -45 to-38 21.1 [11] -50 [23] Auto-ignition °C 420 [11] 434 [11] 468 [23] temp. °C 32.8 [29] 78.4 [29] 27.9 [28]	pressure at 38				
Flash point °C -45 to-38 [11] 21.1 [11] -50 [23] Auto-ignition temp. °C 420 [11] 434 [11] 468 [23] Boiling point °C 32.8 [29] 78.4 [29] 27.9 [28]	deg C				
Image: Image and the	Flash point	°C	-45 to-38	21.1 [11]	-50 [23]
Auto-ignition temp. °C 420 [11] 434 [11] 468 [23] Boiling point °C 32.8 [29] 78.4 [29] 27.9 [28]			[11]		
temp. °C 32.8 [29] 78.4 [29] 27.9 [28]	Auto-ignition	°C	420 [11]	434 [11]	468 [23]
Boiling point °C 32.8 [29] 78.4 [29] 27.9 [28]	temp.				
	Boiling point	°C	32.8 [29]	78.4 [29]	27.9 [28]

Table 4. Physical and chemical properties of fuels

The conducted research, due to its basic character, is aimed at identification of the air-fuel mixture creation changes during simultaneous injection of both fuels. In this research only the conditions of combustible spray build-up in the spark plug area are analyzed. The charge creation conditions were analyzed mainly in the aspect of the time required for the creation of combustible mixture as well as spacious relations in the combustion chamber concerning the fuel sprays' range. Due to the assumed method of fuel supply (direct injection with outward-opening injectors) the mixture creation is being considered through the fuel movement (*spray-guided*). Because of this, the assumed fuel injection is at $685^{\circ}CA$ (35° before TDC).

The stoichiometric mixture creation was based on the assumption, that in dual-fuel injection, this coefficient is referred to the value for gasoline. Thus during ethanol or iso-pentane injection the air demand for these fuels' combustion was not included.

The fuels' spray analysis with two injectors participating begun with simultaneous injection of gasoline only (Fig. 7). The fuel spray analysis was conducted in the range from the start of injection to the point of piston's TDC. The area around the spark plug was subjected to research (the section of combustion chamber was selected to allow for the observation of the fuel spray) referred to fuel droplets distribution and air excess ratio of the A/F mixture (defined as equivalence ratio). The gasoline injection and spray effects in uniform A/F mixture creation on both sides of the combustion chamber (diverse areas in Fig. 7 result from the lack of symmetric section of combustion chamber). At 5° CA before TDC the conditions which correspond to the stoichio-



Fig. 7. The development of the gasoline streams in the two-injectors system (combustion chamber section concerns the $1/\lambda$ quantity); the droplet color indicates its type of fuel (gasoline)

Inflammability evaluation of hydrocarbon fuels mixtures formed directly in the combustion chamber

metric mixture flammability are reached (air excess ratio corresponding to the value of 1). The specific position of the injectors in the combustion chamber causes the A/F mixture to not cover the whole combustion chamber. Such distribution of mixture results in the creation of stratified charges, thus allowing for lean mixtures combustion.

The combustion analysis of various fuel mixtures (gasoline and ethanol) implies that the method of creating the mixture is conditioned by its physicochemical properties. Higher density of ethanol, thus lower fuel outflow velocity from the injector nozzle (Figs 8 and 9) results in the retardation of the A/F mixture creation for this fuel. Thus, the gasoline and ethanol mixture creation should be more effective compared to gasoline only. Such mixture creation characteristics was observed during the analysis of gasoline and ethanol injection (Fig. 10).



Fig. 8. The effect of the initial fuel droplet density during outflow from the injector on the fuel type during injection



Fig. 9. The effect of the initial fuel droplet velocity during outflow from the injector on the fuel type during injection

The analysis of dual-fuel spray (gasoline and ethanol) points to the gasoline spray reaching the spark plug area quicker. In addition, the spayed ethanol remains more compact, because the created mixture covers much less space in the initial spraying period than the gasoline-air mixture. This indicates that the mixture creation in the spark plug area (the air excess ratio enhancing flammability) including gasoline and ethanol is performed with a significant gasoline advance. To minimize these differences, a correction would be required for the injection timing of ethanol.















Fig. 10. The development of the gasoline (red spheres) and ethanol (blue spheres) streams in the two-injectors system (combustion chamber section concerns the $1/\lambda$ quantity



Fig. 11. The development of the gasoline (red spheres) and iso-pentane (green spheres) streams in the two-injectors system (combustion chamber section concerns the 1/ λ quantity

The injection of isopentane, whose physicochemical properties are different from previous fuels, will result in different spray. The isopentane density is lower than that of gasoline, meaning that its mixing with air already starts after a few degrees of CA from the injection initiation. The isopentane spray area is significantly larger than the area of gasoline spray (Fig. 11). In the area of spark plug at 5° CA before TDC the isopentane dictates what flammability point of the mixture will be achieved. Its evaporation at this time is significantly higher than of gasoline as can be seen on the section of combustion chamber around the spark plug.

Based on the above analysis it was determined, that the injection and mixing of both fuels directly before ignition lets spatially shape the air excess ratio in the spark plug area. The injection of two different fuels significantly changes these relations.

5. Fuel mixing analysis

Successive analysis conducted in this area concerns the quantitive coefficients of mixture creation. They contain the global values of analyzed variables. Due to the various values of injected fuels evaporation enthalpy, the temperature values inside the cylinder are subject to changes (Fig. 12). The temperature value change at gasoline and ethanol injection is approximately 3 K (circa 0.5% difference at 715° CA, indicating theoretical ignition point) versus gasoline-only injection. Even higher temperature changes were noted during gasoline and isopentane injection. In this case the temperature drop is of 10 K was registered, and its share is about 2%. These are the mean values related to the whole combustion chamber, which points to significant temperature drop around the spark plug area.



Fig. 12. The cylinder pressure and temperature value course during compression and decompression strokes

Diverse coefficients of fuels' spray are the result of their properties. Due to its lower density, isopentane shows a greater range in typical fuel injection phase (up to 715° CA) (Fig. 13), what was confirmed in spatial research of the atomized fuel spray. The value of isopentane spray range is higher at about 8%, and of ethanol at 2% versus that of gasoline (at 715° CA).

In following part of the spraying process the range decreases, because a significant part of the isopentane fuel dose already evaporated.

The analysis of the absolute value of these fuels evaporated mass confirms the previous results (Fig. 14). It was stated that the mass of evaporated fuels (gasoline and ethanol) is 31% lower than the evaporated mass of gasoline alone, whereas the mass of evaporated fuels: gasoline and isopentane is 31% higher than the evaporated mass of gasoline. Absolute mass values of evaporated fuels point at the twice as high value of evaporated gasoline and isopentane (20.9 mg) versus evaporated gasoline and ethanol (10.8 mg). The amount of evaporated gasoline is at 14.3 mg.



Fig. 13. The effect of the fuel stream range changes on the fuel type during injection and spray to the combustion chamber

Obtained results of evaporated fuel mass allow to determine its total share in injected fuel dose. At 715° CA the shares of evaporated mixtures are:

- a) gasoline 32%
- b) gasoline and ethanol -18%
- c) gasoline and isopentane 34%.



Fig. 14. The effect of the evaporated dose quantity in the combustion chamber on the fuel type during its injection and spray

This implies that mixing fuels before ignition allows for reducing the fuel evaporation speed by 25% (gasoline and ethanol) or increasing this speed by 46% (gasoline and isopentane) versus the standard gasoline injection. This means that gasoline-isopentane mixture lets achieve almost double (92%) the evaporated mass than the gasoline-ethanol mixture.

The analysis of the above results allows to determine the amount of evaporated fuel during injection (Fig. 15). Due to the gasoline-ethanol mixture properties, its evaporation is the slowest and during injection 2% less fuel evaporates than during gasoline-only injection. The gasolineisopentane mixture evaporates quicker and at the end of the injection the evaporated fuel value is 4% higher compared to gasoline-only injection (almost 5% to gasoline-ethanol mixture).



Fig. 15. The effect of the unevaporated dose quantity in the combustion chamber on the fuel type during its injection and spray

Different fuel properties mean that it is important to create the fuel mixture before its combustion directly in the combustion chamber. The analysis presented above points to the significance of this issue in the aspect of searching for solutions lowering the fuel consumption and limiting the CO_2 emission.

6. Summary

The paper describes the research conducted in AVL Fire calculation environment, which is focused on a new direct fuel injection solution. The current knowledge about internal combustion initiated by direct injection fuel supply systems was considered and the dual direct injection fuelling system was introduced.

The research concerns the effects of using three different fuels in combination with gasoline for separate direct injection on spray and flammability of the created mixture directly before ignition.

It was shown that it is possible to shape the air excess ratio in the area of the spark plug by injecting different fuels. Isopentane and ethanol injected through a separate injector than the gasoline have various effects on the airfuel mixture in the area of combustion initiation. The quantitative properties of the spray were presented and the effects described.

The air excess ratio value in the spark plug area depends on:

- fuel density its increase causes limitation of the fuel outflow from the injector nozzle, and as a result – the limitation of fuel spray range,
- injection timing of different fuels different fuel properties, which means: enthalpy of evaporation, density, specific heat and stoichiometric A/F ratio cause different flammability condition in the spark plug area.
 Further research directions include:
- various injection crank angles analysis of both fuels in order to find required flammability in the area of spark presence,
- proper injectors positioning in order to find feasible and optimal solution to execute the dual fuel injection,
- effects on combustion by using described fuel supply system in combination with different fuels.

Acknowledgements

The study presented in this article was performed within the statutory research.

Nomenclature

A/F	air-fuel ratio
CA	crank angle
CI	compression ignition
CNG	compressed natural gas
DI	direct injection
LPG	liquified petrolum gas

Bibliography

- [1] ALEIFERIS, P.G., VAN ROMUNDE, Z.R. An analysis of spray development with iso-octane, n-pentane, gasoline, ethanol and n-butanol from a multi-hole injector under hot fuel conditions. *Fuel.* 2013, **105**, 143-168.
- [2] ARGACHOY, C., PIMENTA, A.P. Phenomenological model of particulate matter emission from direct injection diesel engines. *Journal of the Brazilian Society of Mechanical Sciences and Engineering*. 2005, 27(3).
- [3] ASAY, R., SVENSSON, K., TREE, D. An empirical, mixing-limited, zero-dimensional model for diesel combustion. *SAE Technical Paper*. 2004, 2004-01-0924.
- [4] ASHGRIZ, N. Handbook of atomization and sprays. Springer, New York 2011.
- [5] AVL Fire 2014.2, AVL AST Documentation.
- [6] CAMEO Chemicals. cameochemicals.noaa.gov (accessed 19.03.2017).
- [7] CHEN, Z., GU, F., HU, W. Chemical engineering thermodynamics. *Chemical Industry Press*, Beijing, 2006.
- [8] CHEN, H., REUSS, D.L., SICK, V. Analysis of misfires in a direct injection engine using proper orthogonal decomposition. *Experiments in Fluids*. 2011, 51.
- [9] DECHOZ, J., ROZÉ, C. Surface tension measurement of fuels and alkanes at high pressure under different atmospheres. *Applied Surface Science*. 2004, 1-4(229), 175-182.
- [10] DEMIREL, Y. Energy, green energy and technology. Springer-Verlag London, 2012.
- [11] ELFASAKHANY, A. Investigations on performance and pollutant emissions of spark-ignition engines fueled with nbutanol-, isobutanol-, ethanol-, methanol-, and acetonegasoline blends: A comparative study. *Renewable and Sustainable Energy Reviews*. 2017, **17**, 404-413.
- [12] FOURNIER, S., SIMON, G., SEERSET, P. Evaluation of low concentrations of ethanol, butanol, BE, and ABE blended with gasoline in a direct-injection, spark-ignition engine. *Fuel.* 2016, **181**, 396-407.
- [13] GARG, P., KUMAR, P., SRINIVASAN, K., DUTTA, P. Evaluation of isopentane, R-245fa and their mixtures as working fluids for organic Rankine cycles. *Applied Thermal Engineering*. 2013, 1-2(51), 292-300.
- [14] HUANG, Y., HONG, G. Investigation of the effect of heated ethanol fuel on combustion and emissions of an ethanol direct injection plus gasoline port injection (EDI + GPI) engine. *Energy Conversion and Management*. 2016, **123**, 338-347.
- [15] HUANG, Y., HUANG, S., HUANG, R., HONG, G. Spray and evaporation characteristics of ethanol and gasoline direct injection in non-evaporating, transition and flash-

Maciej Sidorowicz, MEng. – Faculty of Machines and Transport at Poznan University of Technology.

e-mail: Maciej.Sidorowicz@doctorate.put.poznan.pl



- me fuel mass evaporated
- m_r fuel mass remaining
- S penetration
- SI spark ignition
- T temperature
- TDC top dead center

boiling conditions. *Energy Conversion and Management*. 2016, **108**, 68-77.

- [16] JONES, J.J. Hydrocarbons. Physical properties and their relevance to utilization. *C Jones & Ventus Publishing*. bookboon.com, 2010.
- [17] LIU, S, CUTY CLEMENTE, E.R., HU, T., WEI, Y. Study of spark ignition engine fueled with methanol/gasoline fuel blends. *Applied Thermal Engineering*. 2007, 27(11-12), 1904-1910.
- [18] LUCCHINI, T., D'ERRICO, G., ONORATI, A., BONAN-DRINI, G. et al. Development and application of a computational fluid dynamics methodology to predict fuel–air mixing and sources of soot formation in gasoline direct injection engines. *International Journal of Engine Research*. 2014, 5(15), 581-596.
- [19] MOOSAVI, M., DANESHVAR, A., SEDGHAMIZ, E. et al. Shear rate-, temperature- and composition-dependencies of viscosity behavior of mixtures of {[bmim]NO3+ethanol}. *Journal of Molecular Liquids*. 2017, **199**, 257-266.
- [20] PIELECHA, I. Modeling of gasoline fuel spray penetration in SIDI engines. *International Journal of Automotive Technology*. 2014, **15**(1), 47-55.
- [21] Refining online. www.refiningonline.com (accessed 19.03.2017).
- [22] SCHIFTER, I., GONZÁLEZ, U., GONZÁLEZ-MACÍAS, C. Effects of ethanol, ethyl-tert-butyl ether and dimethylcarbonate blends with gasoline on SI engine. *Fuel.* 2016, 183, 253-261.
- [23] Shell Chemicals, Isopentane Q1111, www.shellcom (accessed 19.03.2017).
- [24] SHEN, C., LI, X.-M., LU, Y.Z., LI, C.X. Effect of ionic liquid 1-methylimidazolium chloride on the vapour liquid equilibrium of water, methanol, ethanol, and {water + ethanol} mixture. *Journal of Chemical Thermodynamics*. 2011, 43(11), 1748-1753.
- [25] STORCH, M., KOEGL, M., ALTENHOFF, M. et al. Investigation of soot formation of spark-ignited ethanol-blended gasoline sprays with single- and multi-component base fuels. *Applied Energy*. 2016, **181**, 278-287.
- [26] Thermal-Fluids Central, www.thermalfluidscentral.org (accessed 20.03.2017).
- [27] TURNS, S.R. An introduction to combustion: concepts and applications. *McGraw-Hill*, New York 1996.
- [28] WEI, J. Molecular symmetry, rotational entropy, and elevated melting points. *Industrial & Engineering Chemistry Research.* 1999, **38**(12), 5019-5027.
- [29] ZHUANG, Y., HONG, G. Primary investigation to leveraging effect of using ethanol fuel on reducing gasoline fuel consumption. *Fuel*. 20132, **105**, 425-431.

Ireneusz Pielecha, DSc., DEng. – Faculty of Machines and Transport at Poznan University of Technology.

e-mail: Ireneusz.Pielecha@put.poznan.pl

