Design Concept of Biodiesel Direct Injection Constant Volume Combustion Chamber

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Abstract

This research presents in-house design of the constant volume combustion chamber (CVCC) for observation of diesel conditions at top dead center (TDC), where combustion of injected diesel can be simulated. The system consists of a combustion chamber for combustion of diesel fuel, a mixing tank for controlling the mixture of air (O_2 and N_2) and fuel gas (C_2H_2), as well as initial pressure before being transferred to the combustion chamber, and a gas supply with safety systems to prevent the danger from gas explosion. The constant volume combustion chamber was designed and analyzed by recourse to computer aided engineering (CAE) software Solidworks Simulation. Thermodymics of fuel combustion were analyzed to ensure the strength and safety prior to the fabrication of combustion chamber. Other considerations were taken into account for the use of this constant volume chamber with biodiesel fuel.

Keywords: Constant Volume Combustion Chamber (CVCC), Diesel engine, Computer Aided Engineering (CAE), biodiesel

1. Introduction

The fossil fuels have played a crucial role in the world economy and world energy market. Currently, modern industrial economies rely critically on fossil fuels to supply energy for transportation and to produce electricity for industrial and household purposes [1]. The growth in energy demand or the increase in fossil fuel consumption is stimulated by many factors; predominant among them are the world population growth, economic growth, and the industrialization of developing countries or the continuous industrialization in developed countries [2]. Needless to say, alternative fuel resource has received much interest recently, especially during the fossil fuel price hike. Among other options, biodiesel has been introduced as a blend in diesel. The combustion phenomenon in diesel engine using biodiesel as alternative fuel has been deemed important for understanding thoroughly combustion phenomena and characteristics of free spray combustion. To achieve this, Constant Volume Combustion Chamber (CVCC) has been valuable tools for researchers to understand the complexity of spray and combustion process powering the diesel engine or compression ignition engine (CI).

The safety system of CVCC visualization machine is very important because of very high temperature and high pressure operation condition. The designs of CVCC were published by Daniel [3], Anthony [4] and Rik [6]. However, more detail of design information are still necessary for CVCC development.

This research presents the conceptual design procedure of a constant volume combustion chamber (CVCC) with remark on important equipment, such as gas mixing tank, gas supply system and safety requirement for observation and combustion from computer simulation data.

2. Concept of constant volume combustion chamber as optical rig

Many types of optical test rig are available for simulation of the spray and combustion in diesel combustion, such as Rapid Compression

Machine (RCM), Constant Pressure Flow Rig (CPFR), Constant Volume Hot Cell (CPHC) and especially Constant volume combustion chamber (CVCC) or Constant Volume Pre-Combustion cells (CVPC). From the typical ranges of pressure and temperature in diesel combustion shown in Fig. 1, the combustion pressure and temperature need to be between 4.5 to 15 MPa and between 750 to 950 K, respectively, with gas density between 20 to 60 kg/m^3. Of course, this required operating range would depend on load and compression ratio (CR) but CVCC is designed to cover condition at TDC [6].

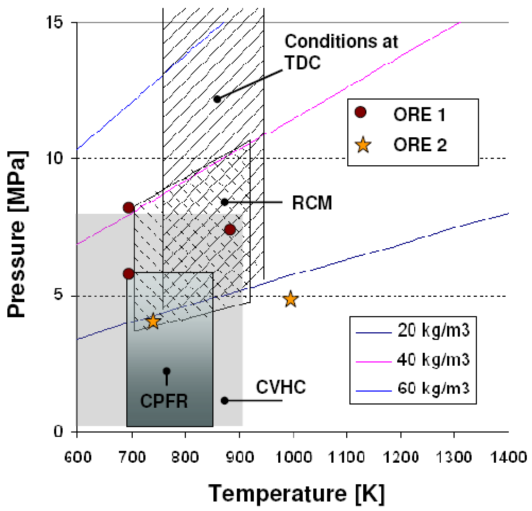


Fig.1 In cylinder condition during diesel injection conditions with different the optical tools [6].

Nonetheless, disadvantage of CVCC is relatively longer time required between measurements, possibly larger in homogeneity of the charge temperature than real engine, and some difference in pressure history during combustion and fuel air-mixing from a real engine.

Diesel combustion conditions using a CVCC are simulated by two stages combustion phenomena, as shown in Fig 2. Firstly, lean premixed gas composed of Acetylene (C_2H_2), Oxygen (O_2) and Nitrogen (N_2) is supplied to CVCC and ignited by spark plug. The mixture is then burned to generate high temperature and pressure combustion condition. Combustion pressure decreases with time after ignition since heat of the flame is lost to the surrounding, which is called the cool down process. The residual gas condition is then suitable for auto ignition in diesel combustion process. Secondly, when combustion pressure has decreased to targeted pressure, the diesel fuel is injected. The data prior to the targeted pressure with diesel injection duration is recorded for analysis on the effect of initial conditions. In this study, combustion pressure of 4.5 MPa is selected according to the combustion ratio of 18 in the isentropic combustion process for comparison with conventional diesel engine.

While previous research has focused on the required ignition of gas combustion delay less than 2 ms of gas combustion in first step with combustion temperature of 950 K and gas density 20.4 kg/m^3 [7]. For the second step, combustion temperature is 750 K at pressure of 4 and gas density of 25 kg/m^3 MPa [5]. Both of reports show the necessary residual O_2 of 10-21% mol for ignition diesel fuel, the present work offers another operating condition.

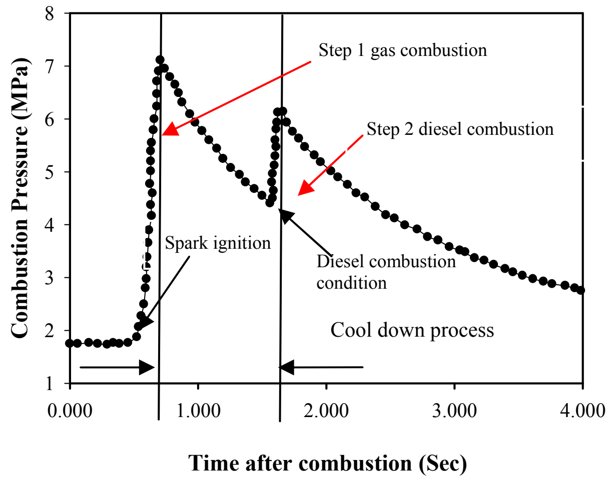


Fig.2 Historical pressure data of two stage combustion for simulated diesel combustion conditions. [6]

3. Theory

3.1 Chemical reaction of combustion

The reaction conditions of diesel combustion can be simulated by pre-combustion of lean premix gas composed of acetylene (C_2H_2) oxygen (O_2) and nitrogen (N_2). Premixed gas combustion can generate high enough temperature and pressure for diesel combustion conditions. Residual product after gas combustion can be simulated as air environment for injection of diesel [6].

$$\underbrace{C_2H_2 + \tfrac{5}{2}O_2 + N_2}_{\text{Premixed gas combustion}} \xrightarrow{\text{Combust}} \underbrace{O_2 + N_2 + 2CO_2 + H_2O}_{\text{Simulated air}} \quad (1)$$

3.2 Real gas mixtures for prepare initial pressure

Controlled premixed gaseous composition for pre-burn gas is important to define. The

Dalton's law was selected as governing equation to calculate partial pressure as shown in eq. 2. For more accuracy, compressibility of gas mixture was selected from partial pressures for high pressure gas mixtures [8] in each gas as shown in eq. 2-6 [9].

$$PV = Z,_{tot} NR_u T \quad (2)$$

$$Z,_{tot} = (a * Z_a) + (b * Z_b) + (c * Z_c) + \\ .... + (n * Z_n) \quad (3)$$

$$P,_{Za} = (a * za * P) / Z,_{tot} \quad (4)$$

$$P,_{zb} = (a * zb * P) / Z,_{tot} \quad (5)$$

$$P,_{zc} = (a * zc * P) / Z,_{tot} \quad (6)$$

When $P,_{Za}, P,_{Zb}, P,_{Zc}$ are corrected partial pressures of the gas. Constant *a, b, c, ..., n* are concentration of the specific gas compressibility factors at different pressures. Z_{tot} is compressibility factor for the gas mixture.

3.3 Lower Flammability Limit (LFL)

After pre-burn combustion, residual O_2 is important for auto-ignition of incoming diesel injection. To ensure enough O_2 would remain, lower concentration of pre-burn gas (especially C_2H_2) can be calculated from lean mixture as Lower Flammability Limit (LFL), shown in eq. 7. The lean limit calculation is obtained from Le Chatelier [10].

$$LFL(\%) = \frac{c_p, N_2 \Delta T_{ad}}{-\Delta h_c} \quad (7)$$

Where

c_p, N_2 is Specific heat of Nitrogen,

ΔT_{ad} is Adiabatic flame temperature,

Δh_c is Combustion enthalpy.

3.4 Adiabatic flame temperature

When the combustion process takes place adiabatically with no shaft work, the temperature of the products is referred to as the adiabatic flame temperature. This is approximately the maximum temperature that can be achieved by balancing between product and reactant in eq.8 [11]

$$\sum_{Prod} N_i (h_f + \Delta h)_i = \sum_{React} N_i (h_f + \Delta h)_i \quad (8)$$

When h_f is enthalpy change and Δh is difference in enthalpy.

4. Design concept results and discussion

The design criteria in constant volume combustion chamber and mixing tank can be discussed as follows. First, all parts of CVCC must be resistant to high pressure during combustion process estimated from simulation results. Second, careful disassembly and assembly of the quartz disc during cleaning must be observed to avoid any minute damage. All parts of gas mixing tank must withstand high premixed gas pressure at target pressure. The gas supply system must be cut off after finish filling gas from mixing tank to CVCC, and must protect explosion of mixing tank when back-firing.

4.1 Concepts of gas combustion calculation.

The calculation of gas combination is to ensure the peak combustion temperature and pressure prior diesel injection, as shown in Fig. 2. This calculation yields the peak combustion pressure for checking with the gas mixture composite and limit for relief pressure of rupture disk. Procedure of gas combustion calculation is shown in Fig 3 with more explanation as follows.

First, review of previous research gives thermodynamic conditions of diesel combustion with the temperature between 850 to 1200 K and pressure is 45 bars. Seconds, trial the premix gas mole fraction (O_2, N_2 and C_2H_2) to obtain enough residual O_2 for ignition at diesel combustion. Third, calculate the adiabatic flame temperature from the mixture as the highest temperature in flame reaction. After obtaining combustion temperature, define the mass (initial pressure of gas composition) in the reaction with ignition gas mixture to get combustion pressure. Forth, when obtaining the lower combustion temperature and pressure under diesel combustion condition, repeat the calculation with the gas mol fraction and initial pressure in step 2 and 3.

From Fig. 4, percent mol of CO_2 increases with increasing percent mol fraction of C_2H_2 since carbon atom in C_2H_2 is changed to CO_2 emission. In addition, with increasing percent of oxygen concentration 10, 13, 15 and 21% after pre burn combustion, percent of CO_2 remains constant. Fig. 5 calculates lower limit for lean quantity of C_2H_2 and air to ensure lean ignition. Given that LFL from Eq. 3 is 2.5 %, LFL at C_2H_2 mixture of 3.5 and 4% are higher. However, with gas mixure of 2.31, LFL is lower than LEF because of lower percent of fuel for reaction.

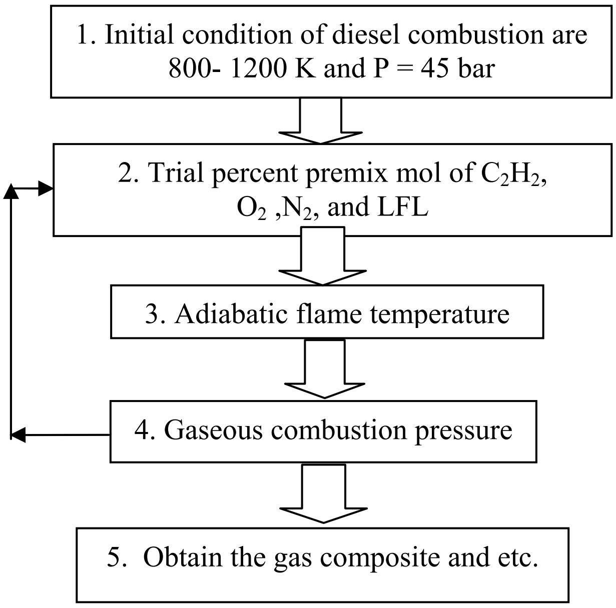


Fig. 3 Procedure to achieve diesel combustion conditions with premix gas combustion.

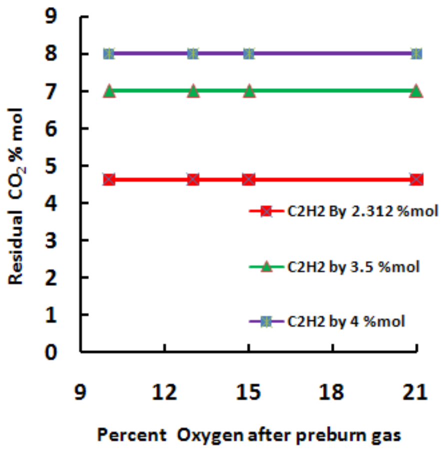


Fig. 4 Percent of CO_2 from various percent oxygen after pre-burn gas with different percent fraction of C_2H_2.

Table. 1 Mole percentage of each pre-burn gas composite.

Before premixed gas burn (%mol)			After premixed gas burn (%mol)			
C_2H_2	O_2	N_2	O_2	N_2	H_2O	CO_2
3.5	29.75	68.5	21	68.5	3.5	7
3.5	23.75	74.5	15	74.5	3.5	7
3.5	21.75	76.5	13	76.5	3.5	7
3.5	18.75	79.5	10	79.5	3.5	7

Table 1 shows the mole percentage of each premixed gas before and after burned conditions. The remaining constant amount of CO_2 and H_2O can be controlled by varying amount of premixed O_2 with the constant mole fraction of C_2H_2. To optimize chemical composition for the mixing gas, C_2H_2 with percent mol of 3.5 was selected with the following reasons: The first reason, C_2H_2 percent mol of 2.312 was lower than the standard LFL (red line in Fig 5), where the gas mixture offers to ignite. The second reason is lower percent of CO_2 after burned gas mixture of 4 C_2H_2 percent moles. In addition, this value is comparable with Sandia [12] and H.gen [6] with 7% mol at percent residual O_2 of 21. The third reason, the gas composite agreed with previous report on the combustion of this C_2H_2 composite [6] in CVCC.

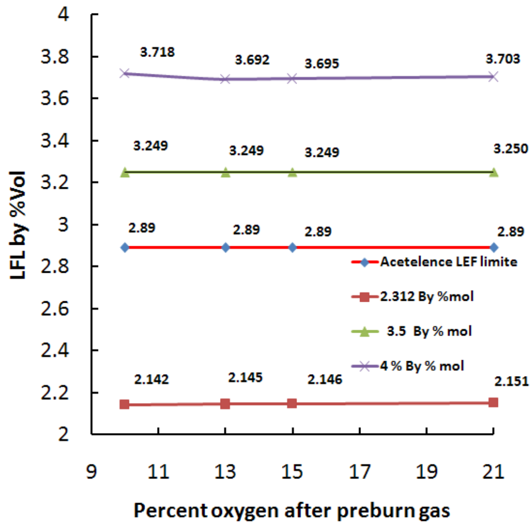


Fig 5. Flammability Limit (LFL) at different percent mol

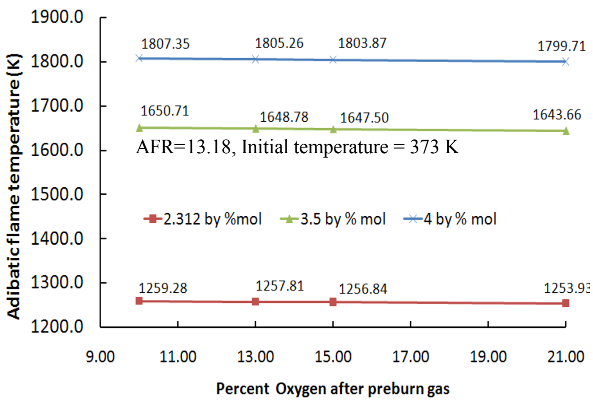


Fig.6 Adiabatic flame temperature with different percent of C_2H_2 and percent of O_2 concentration after combustion.

Fig.6 shows adiabatic flame temperature results, which increase with increasing percent mol of C_2H_2. The results of adiabatic flame combustion is 1799.71, 1643.66 and 1253.90 K for C_2H_2 percent mol of 4, 3.5 and 2.5%, respectively. Absolutely, higher percent mole of fuel reaction results in higher adiabatic flame combustion. It was cleary observed that, the temperature are not increase with very high oxygen concentration of all cases because of enough oxygen amount for chemical reaction.

Next procedure is to trial the prediction of initial pressure to prepare for the gas composite with the partial pressure. Fig. 7 shows results of estimated peak combustion pressure by using the real gas equation with different initial premix gas pressure and percent of O_2. With increasing initial pressure from 5, 10 and 15 bar, the combustion pressure at 21 percent residual O_2 are 22.12, 44.26, and 67.38 bar, respectively. Increase of initial pressure reflects an increased quantity of gas composite for reaction in combustion. After fundamental calculation of chemical composite before and after combustion, Lower Flammability Limit (LFL), Adiabatic flame temperature and peak combustion pressure can be obtained to complete pre-burn gas composition.

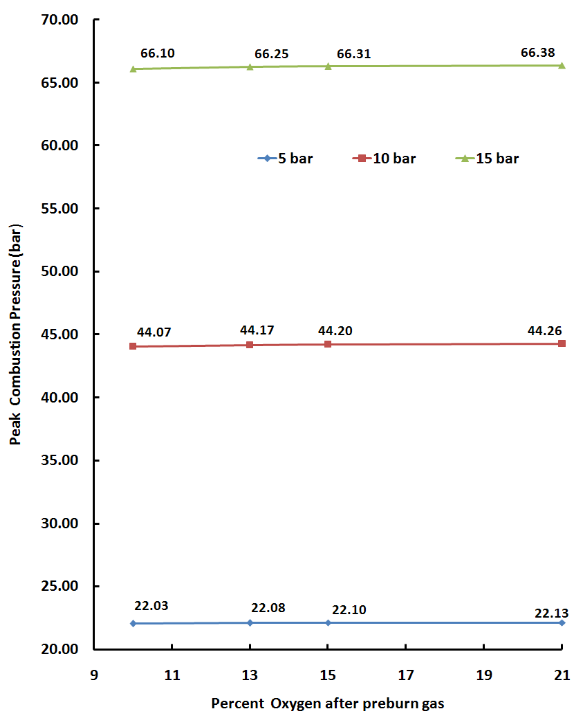


Fig. 7 Peak combustion pressure in different initial combustion pressure

Fig 8 shows partial pressure of premixed gas composite. The C_2H_2 fraction is constant at 0.5 bar but those of N_2 and O_2 are varied for different residual O_2 after combustion. For maximum O_2 of 21% with low N_2 and O_2 of 10%, total gas mixing pressure is 15 bar for conducting an experiment.

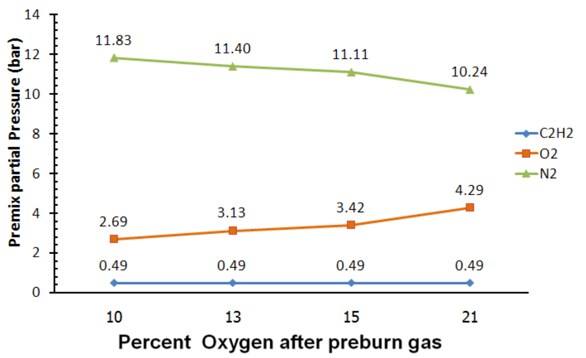


Fig. 8 Partial pressure of preburn gas composition with compressibility (Z) factor at different percent mol of O_2 concentration.

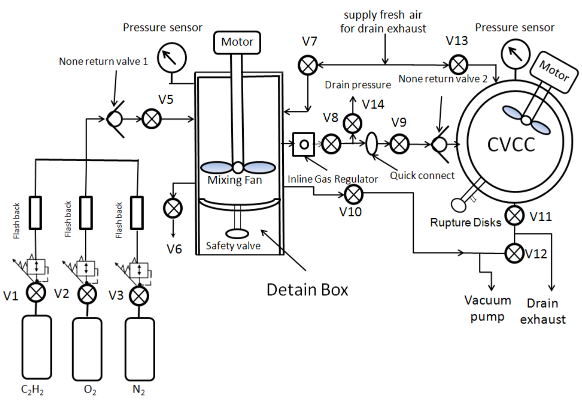


Fig. 9 Schematic gas supply system

4.2 Gas supply system

For premix gas combustion, the gas supply system is important for transferring and measuring of mixing partial pressure of each gas before supplying to CVCC. The concept of gas supply system is shown in Fig 9. Raw gases, C_2H_2, O_2 and N_2, are supplied to premix tank with controlled partial pressure from pressure sensor. Pressure regulator is prepared at 15 bars and supplied to CVCC. Mixture of each gas is maintained by using mixing fan. Safety equipment for gas supply system includes flashback at exit port and safety valve in mixing tank, as schematically shown in Fig. 9. When premix gas pressure is 18 bars, gas is supplied to combustion chamber with reduced pressure. The partial pressure can be controlled by the high resolution pressure sensor. After the premix gas is transferred to CVCC, the gas supply can be disconnect between mixing tank with CVCC by quick conect. Partial gas mixing data is obtained by real gas formula with the gas transfer to combustion chamber. In this design constant volume of combustion chamber (CVCC) is 0.4 Litre for safety concern. For the target pressure of premix pressure in CVCC, pressure regulater is used to reduce to tageted initial pressure of 15 bar. The max pressure in premix tank is defined as the limit of seal and safety equipment.

4.3 Simulation result of mixing tank

Solidworks simulation program version 2012 was used to predict the conditions in mixing tank and CVCC. The simulation assumptions are tri-angular grid sizing of 4 mm., pressure in premix tank of 25 bar, and the surface temperature of 130 degree (the initial temperature of mixing gas). Bond contact was selected for visual bolt fastener support in each part of mixing tank. Material Steel (SS 1035) was selected with the following mechanical properties, yield stress of 340 MPa ultimate tensile stress of 620 MPa . The tank wall thickness is 14 mm.

Fig. 10 shows von mises stress of mixing tank. The curvature of the second part shows around 59.3 MPa with relatively high von mises stress located at the edge of inner hole of 19.5 MPa. Fig 11 shows safety factor being lowest at the inner supply hole of around 2.25 to 3, which agrees to a range of safety of factor for fabrication of the mixing tank.

Fig. 12(a) shows assembly of mixing tank composed of 4 sections. First is the top of tank with mechanical seal of 25.4 mm. diameter for shaft. Second is main tank for installation of gas inlet and outlet port. Third section is lower tank for installation of bearing for mixing fan shaft. The lowest section is installed with safety valve for prevention of tank explosion. Last section is detaining box for protecting relief gas pressure leaving to surrounding by safety valve of 25.4 mm diameter.

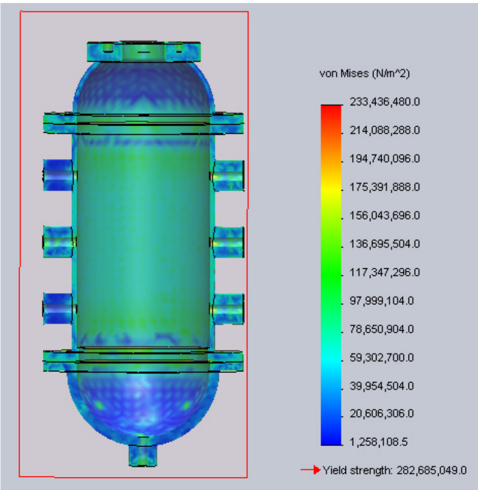


Fig 10 Von mises stress of mixing tank

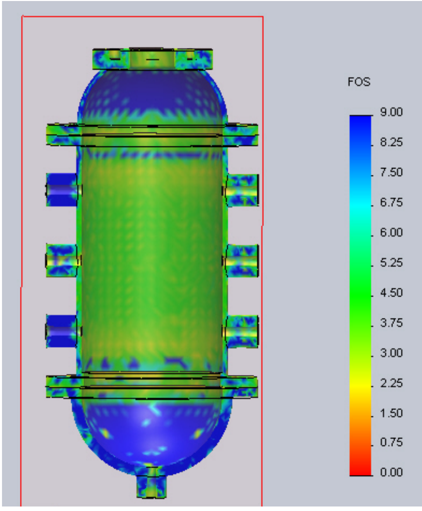
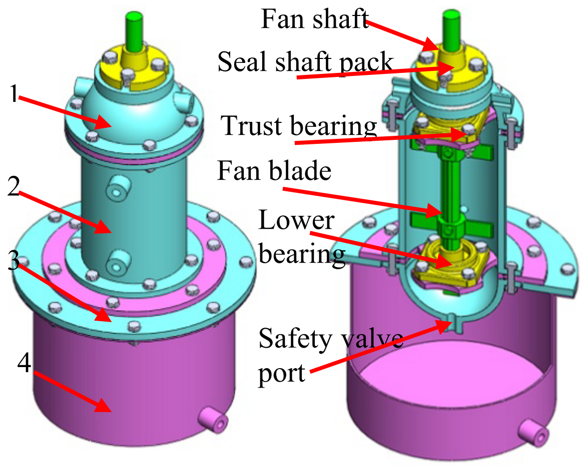


Fig. 11 Safety factor of mixing tank



(a) (b)

Fig 12 (a) Mixing tank layout (b) Section view of mixing tank and detail.

4.4 Simulation results of combustion chamber (CVCC)

Boundary conditions for simulation were selected as tri-angular, base sizing of 4 mm grid. The peak pressure in premix gas is 70 bar, which is higher than estimated calculation pressure in Fig 7. In the simulation, the fixed support components, such as bolt between CVCC and bolt, mixing fan holder, injector pressure sensor, intake valve and outlet valve, assume bond contact. Material is medium carbon steel (S45C) with yield stress of 340 MPa and ultimate tensile stress of 620 MPa.

Fig. 13 shows Von mises stress when applying internal surface with 70 bar pressure. Highest von mises of 47-52.4 MPa is found at hole of spark plug because of stress concentration around the shaft. The outer has von mises stress of around 30 kPa.

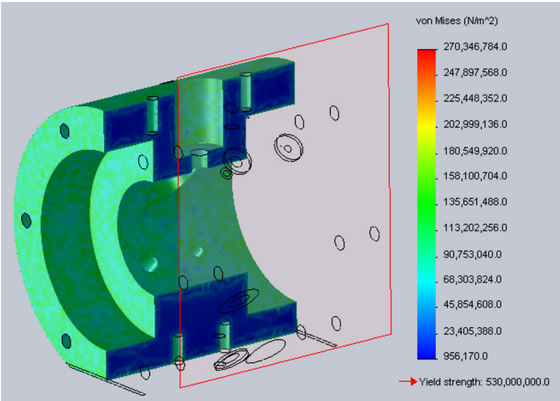


Fig. 13 Von mises stress of CVCC

Fig. 14 shows safety factor of CVCC with reference to von mises stress. The results show that the safety factor at internal section is over 10 and the outer surface is around 4.17 to 5.13. Possible explanation is an effect of thermal stress. Quartz disc is selected for transparent window to observe the flame combustion phenomena in CVCC. Quartz has a diameter of 100 mm, thickness of 35 mm. and edge chamfer of 1 mm. In this simulation, internal pressure of 70 bar is applied with fix support on the opposite side, and thickness from outer diameter of 10 mm. Fig. 15(a) shows von mises stress of quartz being higher at contact with fix support, 31.6 MPa, while other components are around 0.25 MPa.

Fig 15(b) shows that safety factor of quartz is lower at contact with fixed support of 13 while and other component is around 85. From this analysis, it can be ensured that quartz can be used to observe the flame propagation. In order to design quartz holder, PTFE is used to tighten cover in each side surface, which is in contact with quartz holder. To protect edge damage during assembly/disassembly of quartz holder for cleaning optical surface, as well as potential leak, high pressure and high temperature o-ring and graphite are used as shown in Fig.16(a).

Note that all simulation model was validated by conducting a finite element of heavy wall pressure vessel [14] with thin Roak's formula [15]. The results are compared in term of stress in both x-direction and y-direction in element mesh. To check input data of initial boundary condition such as, correct pressure position at acting position, the fix support or reaction.

Furthermore, equipment installed in CVCC is diesel injector, In this experiment, the injector tip with no drilled exit hole is obtained from Denso International Asia with future plan to modify into a single hole at center of injector tip

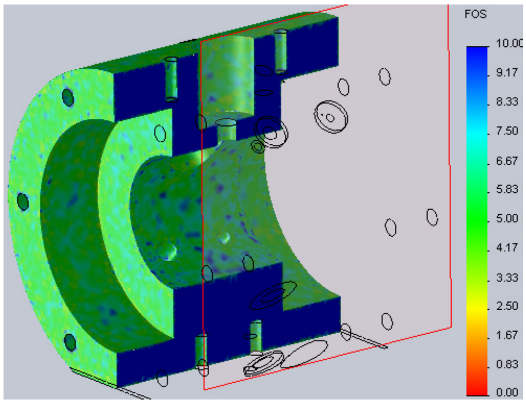
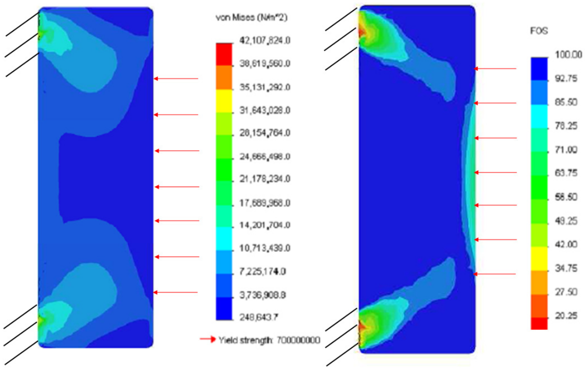


Fig. 14 CVCC safety of factor (FOS)

by micro EDM. Injector cooler keeps constant temperature not exceeding 90 degree as water temperature of the engine. To prevent large change of fuel physical property and thermal expansion of injector needle. Special design of mixing fan with diameter of 28 mm is equipped for uniform gas combustion temperature, before injected diesel fuel.



(a) (b)

Fig. 15 (a) Von mises stress of quartz. (b) safety factor of quartz

A high revolution brushless DC motor of 5000 rpm was selected to drive mixing fan. Seal system between mixing shaft and mixing fan housing are selected with high pressure and temperature polymer seal shaft diameter of 15 mm. Reach ring technique is coupled in mixing fan housing to reduce convective heat transfer from combustion process to seal surface. A rupture disc with bursting pressure of 100 bar is used to vent over combustion pressure at maximum flow area of 23.76 mm^2. Twin band heater of 2,200 Watt is used to heat quartz to avoid water condensing, as well as to increase initial gas combustion temperature.

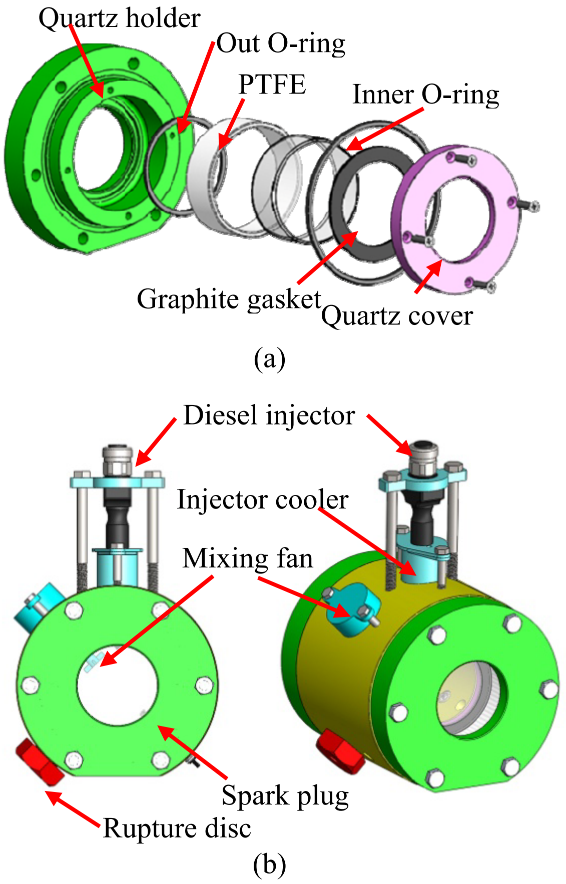


Fig.16 (a) Details of quartz holder with (b) assembly all part of combustion chamber in front and isometric view.

5. Conclusions

The detailed design of constant volume combustion chambers (CVCC) as optical apparatus are presented with safety precaution from simulation and calculation data. The following conclusions were drawn.

Obtain the lean limit, premix gas composite, and regulate partial pressure for proper ignition and combustion to simulate the diesel ambient condition.

Validate the wall thickness, material, shape and position for equipment tools to withstand the high pressure of combustion chamber and mixing tank.

6. Acknowledgement

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