

# Feasibility Study of a Novel Combustion Cycle Involving Oxygen and Water

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## ABSTRACT

A novel combustion cycle which operates in 2-stroke operation and utilizes a novel exhaust valve timing and lift strategy is proposed to potentially replace the existing Otto and Diesel cycles. Air is replaced with oxygen to maximize the combustion efficiency and to enable broader range of fuels to be used. Water is injected into the combustion chamber to enhance the combustion heat absorption, gas expansion and to function as an energy carrier. Engine secondary heat that will otherwise be wasted to the environment is recovered and reused by the engine. Engine theoretical efficiency and out emissions are predicted to be improved.

## INTRODUCTION

The need to reduce air pollutants and to reduce global warming requires drastic actions to be taken. In particular, the source of the problems can be traced back to the inefficiency of the heat engines in converting the hydrocarbon fuels into useful work for power generation and mobility. These heat engines which cover both internal and external combustion engines, waste a lot of energy to the surrounding as secondary heat. Typical internal combustion engines, convert roughly about 1/3 of the chemical energy stored in the hydrocarbon fuels into useful work, the other 1/3 is wasted through exhaust gas and the remaining 1/3 is wasted to the engine coolant [1].

Many new technologies that are related to internal combustion engines have emerged to improve the engine overall efficiency and specific fuel consumption. However, the improvements made are normally minor and do not address the real issue of reducing the heat wasted to the environment.

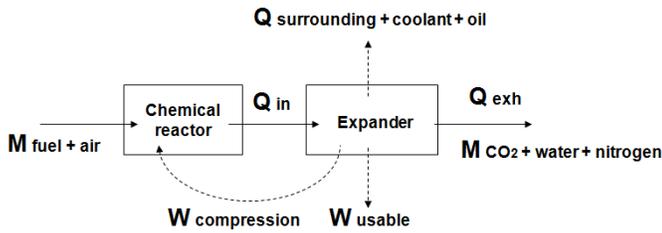
From the perspective of the revised heat engine model, with lesser heat wasted to the environment, the potentials of the engine to do useful work grow larger. Reduction in the heat wasted to the environment is desirable because by cutting the waste into half, global hydrocarbon fuel consumption rate may also be cut by half. This may eventually lead to reductions in greenhouse gases and pollutants productions from the heat engines by half as well.

In minimizing the heat wasted to the environment from heat engines, a novel combustion cycle is proposed which replaces air with water as the main working medium. By using water as the main working medium, it absorbs heat and expands better than air. Remaining heat that is not absorbed during combustion can still be recovered by water at the heat exchangers and reintroduced into the engine using the water as an energy carrier.

Oxygen instead of air accelerates the heat release making it possible for water to be introduced without affecting the flame development. More complete combustion maximizes the combustion efficiency and minimizes the formations of HC, CO and PM. Lack of nitrogen in the combustion ensures very minimum NO<sub>x</sub> formation. The use of oxygen also enables broader range of gaseous and liquid fuels to be used which indirectly minimizes the cost and energy required to process cleaner fuels.

This paper discusses the feasibility of the novel combustion cycle to achieve improvements in terms of theoretical engine efficiency and engine out emissions.

## CONCEPT DEVELOPMENT FROM THE PERSPECTIVE OF REVISED HEAT ENGINE MODEL



**Figure 1: Revised heat engine model for conventional heat engines**

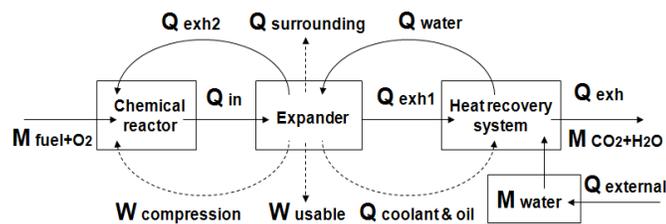
A revised heat engine model as described in Figure 1 is created to represent a typical internal or external combustion engine. The solid line represents a process where mass is transferred. The dash line represents a process where no mass is transferred.

From the revised heat engine model, both air and fuel are delivered into the “chemical reactor” process. The “chemical reactor” process is representative to the combustion chamber where fuel is oxidized to release heat.

In a typical internal combustion engine, the “chemical reactor” represents the combustion chamber with piston at the TDC. The arrow “W compression” represents the compression work required to heat the charge to auto ignite the fuel and air. From the model, air that is used as an oxidizer and a working medium is introduced to the “chemical reactor” process.

Once auto-ignition of fuel has occurred, the released heat will be transferred together with the charge from the “chemical reactor” process to the “expander” process. The “expander” process represents a process where work “W usable” is extracted from the gas expansion during the expansion stroke.

Only about 1/3 of the heat supplied from the fuel oxidation is turned into work while another 2/3 is wasted to the surroundings through exhaust gas, coolant and oil [1]. Significant portion of the generated work is used to compress the charge to provide activation energy for fuel auto-ignition reaction to take place.



**Figure 2: Revised heat engine model involving novel combustion cycle**

As shown in Figure 2, oxygen is delivered to the “chemical reactor” process for fuel oxidation to take place. Water as a working medium for heat absorption and for gas expansion is introduced to the “expander” box at a later stage.

Cylinder temperature is raised for fuel auto-ignition to take place not only by compressing the charge. Instead, significant amount of thermal energy is made available to the “chemical reactor” process by retaining the hot exhaust gas from the previous cycle.

Upon successful fuel auto-ignition, thermal energy is supplied to the “expander” process not only from the fuel oxidation. Instead, heat recovered from the engine exhaust gas, coolant and oil is also delivered into the combustion chamber using heated water as an energy carrier.

These two heat sources increase the amount of heat available to be converted into kinetic energy by the “expander”. Further improvement is also possible by supplying heat “Q external” from external sources like sunlight, brake system, etc. which is again delivered into the engine using heated water as an energy carrier.

With maximum heat available to the expander, the temperature difference between the combustion by-products and the injected water allows rapid heat transfers to take place. Water having high specific heat capacities in both liquid and gaseous forms maximizes the heat absorption. With higher heat absorption, there will be lesser heat rejected as waste heat.

In addition, with higher heat absorption, water changes phase from liquid into vapor very quickly and the heat transfer continues until temperature equilibrium is reached. Injected water having its thermal energy content and enthalpy rapidly increased, expands to push the piston downward.

Theoretically, by making sure that very little heat is wasted, maximum work can be obtained from the “expander”. Furthermore, by supplying external heat into the engine, it is not theoretically impossible for the engine to produce more work than the energy supplied by the hydrocarbon fuel.

From the revised heat engine models, factors that affect the overall engine operation and its efficiency have now been simplified. These factors can now be prioritized and individually improved to maximize the impacts in making improvements to the engine’s overall efficiency.

## REPLACEMENT OF AIR WITH HIGH PURITY OXYGEN

Earlier works in using oxygen enriched air are well documented [2, 3, 4, 5]. These experiments involved oxygen enrichment of up to 40%. The researchers have reported positive results in terms of improvements in

emissions, efficiency and fuel consumption. Although significant improvements have been reported in HC, CO and PM emissions, many have reported significant increase in NO<sub>x</sub> due to increased in peak cylinder temperature resulting in from the use of oxygen enriched air [3, 4, 5].

Researchers in England and Canada have experimented with the use of oxygen for complete replacement of air intended for underwater engine application [6, 7]. The experiments involve the use of either CO<sub>2</sub> or argon to replace nitrogen. The use of 30% oxygen when premixed with 70% carbon dioxide resulted in reduction of engine power by 20-23% and increase of fuel consumption by 23-28% indicating that the carbon dioxide acted as a combustion inhibitor [6]. The results have led the authors to conclude that the carbon dioxide was seriously affecting both the pre- and post-ignition processes [6]. These results have suggested that premixing pure oxygen and carbon dioxide may not be the best way to fully exploit the use of pure oxygen. In this context, the novel cycle avoids the use of oxygen premixing and prefers the use of stratified oxygen and fuel.

Using pure oxygen instead of air reduces total charge to be inducted and compressed by at least 78% if compared to conventional engines running with stoichiometric air-to-fuel ratio. With such a large reduction in total charge inducted, compression work is greatly reduced which eventually leads to lower FMEP. Furthermore, with 78% decrease in the charge mass to be inducted into the cylinder, intake poppet valves can be replaced with gas injectors. This enables accurate and more freedom of operation for the injector independent of engine speed.

For practical application, the use of pure oxygen with purity level of more than 99% necessitates the use cryogenic process using the Joule-Thompson method. Instead, high purity oxygen with purity level in the range of 90-95% generated using pressure swing adsorption (PSA) is preferred as it gives a good balance between oxygen purity and power consumption. The use of PSA process also has other merits like small investment, safety and convenience [8].

In using PSA process for oxygen generation, the remaining impurity consists of argon [9]. Argon being an inert gas does not chemically react before, during and after combustion. Therefore, even if the argon content approaches 10%, it is still acceptable as it will not end up as harmful pollutants. In selecting the right PSA equipment, it is also important for the nitrogen content to be as low as possible. This is to minimize the possibility of the nitrogen gas from being oxidized into NO<sub>x</sub> pollutants during combustion.

As discussed earlier, the use of PSA process is suitable for small and medium scale applications. This enables the PSA generator to be integrated with the fuel refilling

station for onsite oxygen production. This integration eliminates the needs for costly oxygen delivery using tanker or pipeline. Furthermore, there is no need for the refilling station to store large amount of oxygen. Since air inducted for the PSA process is free and readily available at the fuel refilling station, the costs to produce the high purity oxygen mostly comes from the power consumption, operation and maintenance.

In 1990, it is reported that the production of oxygen consumes about 0.36-0.41 kWhr of power for every kg of oxygen [10]. At the time of writing, mass production of high purity oxygen utilizing the latest oxygen generation technology available enables the power consumption to be reduced to as low as 0.21 kWh/kg [11]. The power consumption reduction trend is likely to continue in the future, especially if there are increasing demands for oxygen from the transportation sector. With the possibility of generating high purity oxygen without consuming a lot of energy, the penalty of using high purity oxygen instead of air is much lower than what was previously thought.

Considering that the oxygen generation consumes significant energy, it is crucial for this paper to highlight the significance in energy savings. It has been reported that the oxygen enrichment in Aluminum melting furnaces enables fuel cost to be reduced when the oxygen purity is increased [12]. Praxair's corporate website listed many of the currently available heating technology that utilizes high purity oxygen and the fuel consumption reductions range from 25-60% [13].

Reducing the fuel cost is important in the future considering that there will be constant increase in world's energy demands which is made worse with depleting natural resources. With high purity oxygen, the intense heat release enables lesser fuel to be oxidized to generate the same flame temperature target [14]. The prospect of generating intense heat with low fuel consumption through the use of high purity oxygen fits the supply of heat "Q in" requirement as specified in the revised heat engine model.

The use of high purity oxygen instead of air, enables more oxygen molecules to be available adjacent to the hydrocarbon molecules. With adequate activation energy available to the charge for chemical reaction to take place, increased density of oxygen molecules will accelerates the fuel oxidation process. As a result, ignition delay will be shortened. At the same time premixed combustion is minimized while diffusion combustion is maximized. With the heat release rate greatly increased, it takes much shorter time to complete the entire heat release process.

With such a high heat release rate, the cylinder temperature increase rate is far higher than what is possible with combustion involving air. In terms of flame temperature, fuel oxidation involving oxygen instead of air is expected to increase the flame temperature by

around 500-800K [15]. This necessitates a set of countermeasures to avoid part overheating problems. In controlling the heat release rate and peak cylinder temperature, it is crucial for the fuel injection flow rate to be accurately controlled to avoid sudden heat release in both the premixed and diffusion combustions.

Combination of high heat release rate and high flame temperature is likely to increase the combustion efficiency if compared to what can be achieved in conventional heat engines. Higher combustion efficiency leads to lower HC, CO and PM emissions. Although it is preferable for the engine to operate with stoichiometric combustion to minimize oxygen wastage, operating the engine with equivalence ratio of below 1 may further improve the HC, CO and PM emissions.

In terms of NO<sub>x</sub> emission, other researchers have reported that the enrichment of oxygen in air from 21% to 30% is likely to increase the formation of NO<sub>x</sub> [3, 4, 5]. To overcome the problem, as discussed earlier, the oxygen purity of at least 90% is sufficient to minimize the presence of nitrogen during combustion. With very minimum nitrogen involved in the combustion, it is likely that the formation of NO<sub>x</sub> is also minimized. This enables the increasingly expensive and complicated NO<sub>x</sub> aftertreatment system to be totally eliminated. This in turn will reduce the vehicle's cost, weight and exhaust back pressure. With very minimum NO<sub>x</sub> formation, depending on the engine's peak combustion temperature limit, it may be possible for cylinder temperature limit to be increased from 2000K to 2200K to further enhance the combustion efficiency.

In the context of the revised heat engine model, the use of oxygen provides the best possible solution in maximizing the availability of heat to the expander rapidly, efficiently and effectively. This fits well with the bigger picture of the novel combustion cycle.

## **WATER AS A WORKING MEDIUM**

Water in general is cheap, abundant, renewable, harmless and chemically stable. Specific heat capacities of water in both liquid and vapor forms are much higher than carbon dioxide and nitrogen which normally present during combustion in conventional engines. If water can be made available in the cylinder by the time heat release is about to complete, a lot of heat can be absorbed by the water. Furthermore, the peak cylinder temperature can be accurately controlled by varying both the water mass and temperature.

Earlier work has indicated that the delivery of water prior to the fuel auto-ignition significantly affects the ignition delay [16]. Low temperature too early in the combustion increases engine noise and ignition delay [17], thus it is desirable for charge temperature near the TDC to be maintained above certain temperature. Significant improvement can be made over other prior arts if the water injection is introduced not before the fuel auto-

ignition. In doing so, the charge cooling effect from the water injection does not take place during the compression stroke. Indirectly, compression work required to increase the charge temperature for optimum fuel auto-ignition can be reduced by injecting water at a later stage.

Considering that the oxidation of fuel involving the high purity oxygen releases a lot of thermal energy inside the combustion chamber, some form of cooling agent is required to cool off both the charge and metal surfaces. Water being delivered into the combustion chamber after certain amount of heat has been released can be very effective in cooling the charge and metal surfaces. Although water in cylinder head and cylinder block water jackets is sufficient in cooling the metal surfaces, greater improvement is possible by having water in direct contact with high temperature gases in the cylinder without any metal wall in between.

Earlier work in direct injection of water for cooling the cylinder has shown some encouraging results [18]. The water injection provides direct cooling over hot surface areas covering cylinder liner and piston crown [18]. Using this prior art as a baseline, further improvements in the design details and method of operation may make it possible for water jackets in both cylinder block and cylinder head to be reduced or even eliminated.

The vibration of water molecules gets faster as more combustion heat is absorbed and it continues until the water molecules got separated from one and another. The change of state from liquid to vapor is accompanied by further heat absorption which is also known as latent heat of evaporation. This process further enhances the cooling effect of the water injection as large amount of thermal energy is converted into other form of energy in a very short time period.

Once in vapor form, the water molecules vibrate faster causing more water molecules to collide between one and another. This leads to further increase in pressure of the enclosed volume. For comparison, the individual gas constant  $R$  for steam, carbon dioxide and nitrogen are 0.461 kJ/kg\*K, 0.189 kJ/kg\*K and 0.297 kJ/kg\*K [19]. Assuming that the injected water is fully vaporized, according to the ideal gas law, with every degree Kelvin increase in charge temperature, the steam pressure increase is 2.43 times higher than carbon dioxide and 1.55 times higher than nitrogen.

Carbon dioxide and nitrogen which exist in gaseous state all the time in the engine requires large pipe cross section for the gases to be moved around the engine. Gas having a much lower density in general if compared to liquid, requires it to be compressed to speed up delivery. Furthermore, compression of gas is accompanied with an increase in temperature which is undesirable in terms of energy consumption and flow rate. Often, charge cooling is required to control the gas temperature. Furthermore, the work required to

compress gas to certain pressure is far higher than the work required compressing liquid to the same pressure.

Careful manipulation of water pressure and temperature makes it possible for the specific heat capacity and boiling point to be varied to benefit the engine. For example, as water is compressed from ambient pressure to 150 bar, the boiling temperature increases from 100° Celsius to 342° Celsius [20]. At the same time, the water specific heat capacity is increased from 4.18 J/g\*K to 6.8 J/g\*K [20]. In exploiting these excellent water properties, if water is compressed to 150 bar, a lot of heat can be transferred from hotter region to the compressed water without rapidly increasing the water temperature. The heat transfer can continue until the water temperature is about 320°-330° Celsius without the water vaporizing into steam. At this water temperature and pressure, the energy content and enthalpy are far higher than water at ambient temperature and pressure.

As long as the water is still in liquid state, it can be transported easily using relatively lower compression work and relatively smaller pipe cross section. By moving the pressurized water from one high temperature spot to another, plenty of heat can be scrubbed with minimum investment in terms of the compression work. Heat transfer to the compressed water can occur from any heat source with relatively higher temperature.

If the piping network, pump, valve and other related parts are well insulated, one can transport a lot of energy from one place to another with minimum heat loss. Indirectly, the heated water also functions as an energy carrier. Contrary to that, it is also possible to transport heated nitrogen around but it is not desirable to do so considering the lower mass density and energy content involved require higher pumping work and bigger pipe cross section.

The presence of high amount of water in the exhaust gas can be beneficial in scrubbing sulfur oxides generated in the combustion from the use of high sulfur fuel. By cooling the exhaust gas to certain temperature using a condenser, large amount of water will condensate. As the water condensates, it may be possible for the water to dissolve the sulfur oxides gases into sulfuric acid. This may significantly reduce the amount of sulfur oxides discharge into the environment. Furthermore, the expensive and energy intensive desulfurization process at the refinery may be avoided, resulting in lower well-to-wheel carbon dioxide discharge into the environment.

From the perspective of the revised heat engine model, it is clear that water is a better working medium if compared to both nitrogen and carbon dioxide. Water functions very well in terms of heat absorption, gas expansion and moving the thermal energy around.

## ENGINE DESIGN CONSIDERATIONS

As shown in Figure 3, the combustion chamber layout is designed to have 2 oxygen injectors, a fuel injector and an exhaust valve. The lower part of the combustion chamber consists of 2 water injectors mounted to the cylinder block. The water injectors are purposely designed to point upward as shown in Figure 4. Small opening at the upper portion of the cylinder bore formed using drilling operations enables water delivery into the combustion chamber. The water jacket surrounding the cylinder bore must also be designed to accommodate the placement of the water injector.

This opening is combined with recess at the top outer edge of the piston. As the piston moves downward during expansion stroke, water spray is spread out over a wider area of coverage. This may minimize uneven cooling of the cylinder head flame face.

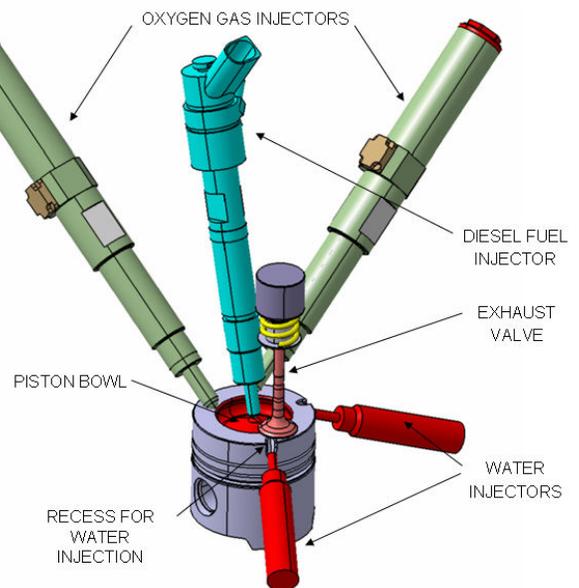


Figure 3: Combustion Chamber Layout

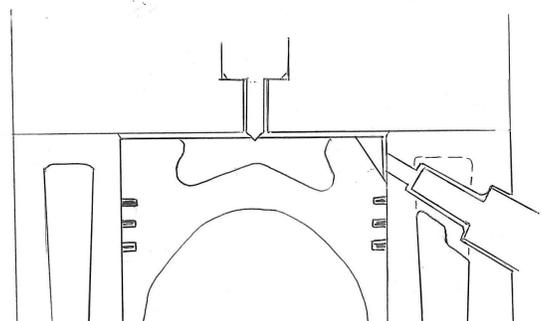


Figure 4: Water Injector Mounting

As shown in Figure 3, the oxygen injectors are positioned in such a way for oxygen to be delivered straight into the piston bowl. Feed pressure of around

200 bar enables powerful blast of oxygen which is crucial considering rapid pressure rise at the TDC.

Common rail DI Diesel injector delivers fuel into the piston bowl similar to conventional Diesel engines but at much lower feed pressure. Stratification of both fuel and oxygen in the piston bowl enhances mixing ensuring good mixture preparation prior to the fuel auto-ignition. Glow plug (not shown) is required to heat up the combustion chamber during start up operation.

Piston bowl, top surface, top land and cylinder head flame face need to be coated with thermal resistance coating. Ceramic coating can be one of the options as it enables the piston to withstand higher combustion gas temperatures [21]. Piston cooling jet is a must in order to cool off the piston bowl area from below using oil squirt.

Piston rings are coated with Diamond-Like-Carbon (DLC) coating to enable high wear resistant and low friction coefficient. This coating is crucial in minimizing wear rate between the piston rings and cylinder bore considering that there may be some water condensation on the cylinder bore surface when the exhaust valve is opens.

Motorized variable valve timing (VVT) from INA is required to enable wider cam phasing if compared to what is achievable from hydraulically actuated VVT [22]. Such motorized VVT is crucial during engine start up. Furthermore, the motorized VVT enables rapid phase change even at low engine speed and oil pressure.

Continuous variable valve lift with a fixed opening duration is needed to enable the exhaust valve lift to be varied without any variation in the opening duration. Such concept is currently being developed and the detail is not yet available to the public.

The rated power is achieved at relatively lower engine speed if compared to conventional engine. This enables low viscosity multi grade engine oil to be used. Nevertheless, the engine oil needs to be able to withstand higher water contamination in the oil sump due to the high water content in the blow-by gas.

### SEQUENCE OF EVENTS

As shown in Figure 5, during engine start up, both exhaust valve closing (EVC) and exhaust valve opening (EVO) is advanced until the EVC point is at the BDC. As the piston moves downward, vacuum is created inside the cylinder. Once the exhaust valve opens, the difference in pressure results in ambient air to be inducted into the cylinder through the exhaust port. To avoid foreign materials from entering the combustion chamber, the catalytic converter temporarily functions as an air filter. Full effective compression ratio is possible during the engine start up. Glow plug is needed to provide additional heating of charge at TDC. Once fuel auto-ignition is achieved, both EVC and EVO points will

be rapidly advanced to its normal position. During the transition period, oxygen injection starts and the amount of oxygen injected gradually increases.

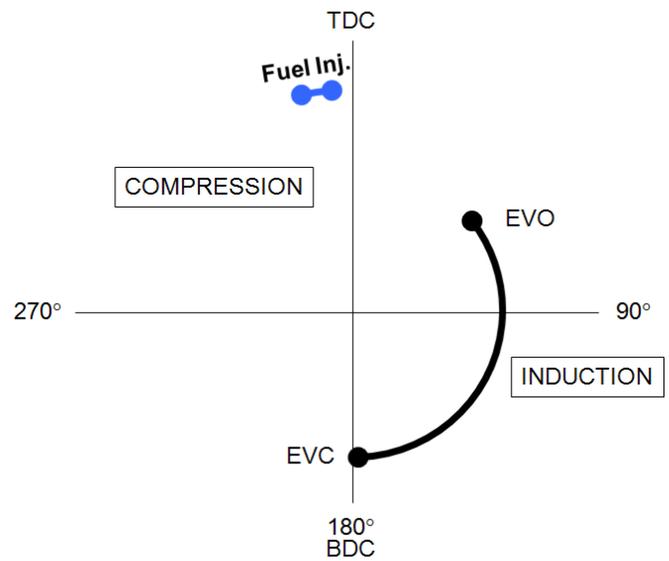


Figure 5: Engine operation during start up

As shown in Figure 6, the EVC and EVO points are back at the normal position after the engine start up sequence. This enables the engine management system (EMS) to switch to the idle operation. At idle operation, the EVO point is about few degree crank angle away from the BDC. There is no need for a long blowdown operation as there is only minimum total charge involves.

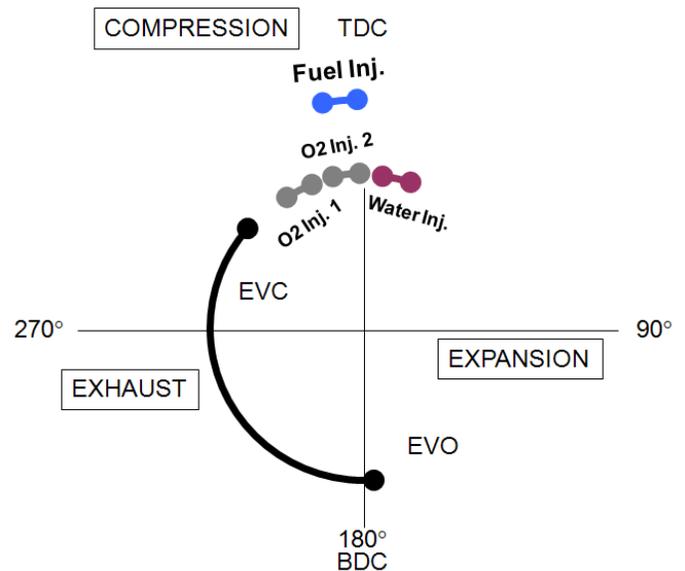
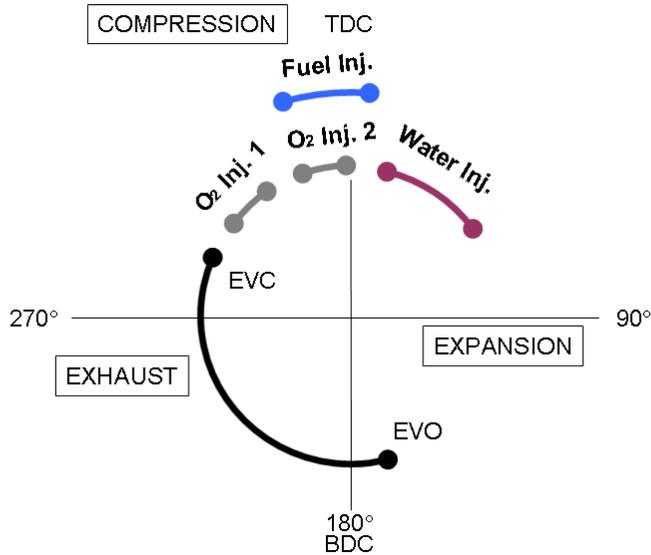


Figure 6: Engine operation during idle

In making sure that the charge is hot enough at TDC for fuel auto-ignition to occur, exhaust valve lift is at its minimum to enable exhaust gas to be throttled. Earlier work in throttling the exhaust gas at the exhaust manifold shows insignificant increase in cylinder

pressure and pumping work [23]. 1D simulation conducted in a separate study using similar exhaust valve lift strategy confirms that the increase in cylinder pressure and pumping work is insignificant [24].

As shown in Figure 7, the EVC and EVO points are slightly advanced if compared to the EVC and EVO points for idle operation. This slight advancement enables longer blowdown period which is necessary at full power especially when it involves larger total charge and higher engine speed.



**Figure 7: Engine operation at full power**

The total water present as the cylinder approaches the TDC must not be more than the clearance volume when the piston is at the TDC. This is to avoid the risk of hydraulic lock that can be damaging to both reciprocating and rotating engine parts. Coordination between the total mass of water injected, exhaust valve timing and lift is necessary to ensure the water content as the piston approaches TDC is below the limit. To further reduce the risk of hydraulic lock, it is not advisable to inject water before the TDC.

With the amount of recoverable secondary heat changes with engine speed and load, the water temperature at the point of injection will also change. Full calibration at various engine speed and load is necessary to ensure that the targeted exhaust gas temperature as the exhaust valve opens is achievable.

### LOWERING THE COMPRESSION WORK

The expansion of oxygen as it exits the gas injector's nozzle results in sudden temperature decrease that may affect the fuel's auto-ignition. Furthermore, with the use of oxygen to replace the ambient air, the total charge involved during compression is relatively lower if compared to conventional engines. To make the situation worse, full compression stroke is not possible

as it is necessary to discharge some of the exhaust gas before the next compression work starts.

Many researches done in the area of HCCI have reported the significance in using residual gas as an option to control the fuel auto-ignition [25, 26]. With higher internal EGR trapped inside the combustion chamber, higher cylinder temperature can be expected leading to earlier fuel auto-ignition [27, 28]. Furthermore, the trapping of the residual gas eliminates the need for high compression ratios or a heater to increase the charge temperature [29].

In the context of this novel engine, the thermal energy in the cylinder increases with higher residual gas trapped in the cylinder. In addition, the remaining water vapor from the previous cycle increases the charge's heat capacity to enable higher residual gas temperature even when significant heat transfer occurs from the residual gas to the surroundings during the exhaust gas discharge.

As it is impossible to rely only on the residual gas to increase the cylinder temperature above the fuel's auto-ignition temperature, compression work is needed to fill the gap. Varying the effective compression ratio by varying the EVC point is necessary in order to control the compression work needed to increase the cylinder temperature to the optimum cylinder temperature for optimum fuel auto-ignition to take place.

With residual gas content as high as 50% in the cylinder, it is necessary for oxygen and fuel to be stratified inside the piston bowl. Without the stratification, the high carbon dioxide content results in deterioration in flame speed and combustion efficiency. Earlier work by Orbital in stratifying fuel with air using air-assisted direct injection is well documented [30]. The author has reported improvements in fuel consumption, combustion stability, HC emission and EGR tolerance of up to 40% [30]. The CFD plot included in the paper has also suggested that the injections of air and fuel into the piston bowl replace most of the residual gas in the piston bowl with fresh charge of air and fuel [30]. In this context, the novel cycle relies on the use of stratified oxygen and fuel in the piston bowl to ensure optimum flame development even with high residual gas content in the cylinder.

It is also interesting to point out that as this novel engine operates only in 2-stroke, double charge compressions as described by Santoso in his thesis [31] can be avoided. The double charge compression brings about many undesirable effects in using the early exhaust valve closing strategy to exploit the use of residual gas in controlling the fuel auto-ignition in 4-stroke HCCI.

### 1D AND 3D SIMULATIONS

To evaluate the potentials of the novel cycle, both 1D and 3D are used. The use of 1D simulation using LMS AMESim IFP-Engine is effective in conducting parameter

optimizations for the 3D boundary conditions. Understanding that the 1D simulation has limitations in predicting the thermodynamics aspect of the engine in 3-dimensional, 3D simulation has to step in to fill the gap.

The 3D simulation involves the use of LMS AMESim IFP-C3D version 1.3.0. The use of 3D simulation enables predictions in fluid dynamics, chemical reactions, heat release, heat transfer, etc. Many of the 3D simulation outputs are fed back into the 1D simulation through series of iterations.

Combustion heat release rate in the 3D simulation is simulated using Barba's method [32, 33]. The 3D simulation starts as the exhaust valve is fully closed and it is completed just before the exhaust valve starts to open.

With both 1D and 3D simulations play an important role in the research, a baseline engine design involving less than optimum engine design parameters were used. This enables sensitivity analysis to be made as design parameters are improved from time to time.

A set of 3D models consisting of piston top, combustion chamber flame face, exhaust valves, fuel injector, water injectors are used in the simulation. The assumptions made are listed below: -

- 1) The bore and stroke are assumed to be 66mm and 80mm.
- 2) The geometrical compression ratio is assumed to be 16.
- 3) Light Diesel fuel is used with 1600 bar fuel injection pressure
- 4) Oxygen purity is assumed to be 95% with the remaining 5% being nitrogen
- 5) The engine speed is fixed at 2000 rpm.
- 6) Residual gas amount retained in the cylinder is assumed to be 40%.
- 7) Water is injected at 5.5:1 water-to-fuel ratio with feed pressure and temperature of 120 bar and 363K
- 8) Cylinder temperature at the point of fuel auto-ignition is fixed at 1000K
- 9) Equivalence ratio of 1

The novelty of the novel cycle limits the availability of commercially available software to fully simulate the cycle. Classical calculations were used to compliment the software used. Special codes may have to be developed in the future and correlated with the actual physical testing.

## RESULTS AND DISCUSSIONS

In general, the expansion ratio for the novel cycle is relatively longer if compared to conventional 2-stroke engines. The use of oxygen instead of air reduces the overall charge mass thus the EVO point can be significantly retarded closer to BDC if compared to EVO point of the conventional 4-stroke engines.

The EVC point can be advanced and retarded to change the effective compression ratio and residual gas trapping. Advancing the EVC point increases the effective compression ratio resulting in higher compression work and residual gas trapping. Retarding the EVC reduces the effective compression ratio resulting in lower compression work and residual gas trapping.

While the exhaust valve timing is varied, the lift will also be varied to throttle the discharge of exhaust gas into the exhaust port. Exhaust valve lift as low as 1mm is used at idle while maximum valve lift is used at full power. Varying both the exhaust valve closing point and lift is crucial in accurately controlling the cylinder temperature near the TDC for optimal fuel auto-ignition. Furthermore, accurate cylinder temperature at TDC avoids excessive compression work and cylinder temperature increase. In theory, multiple fuel operation using a single engine is possible as the cylinder temperature near TDC can be accurately varied to suit the various fuel auto-ignition temperatures.

Once the EVC point is reached, oxygen is delivered into the combustion chamber using the oxygen injector. Powerful blast generates swirl with a swirl ratio of around 14 as shown in Figure 8. The blast also displaces the residual gas inside the piston bowl elsewhere. This is followed by fuel injection into the piston bowl to complete the stratification of both fuel and oxygen. High swirl ratio and the stratification of both fuel and oxygen enable better mixture preparation.

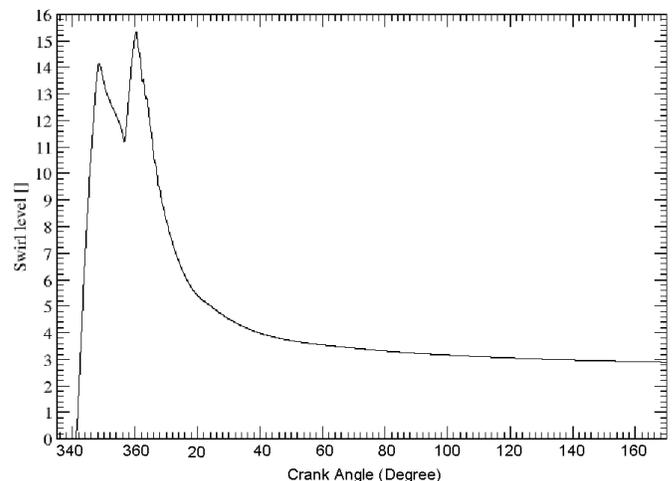
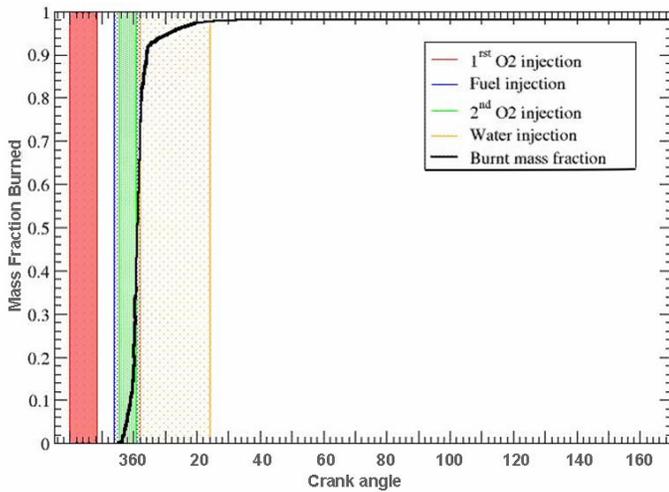


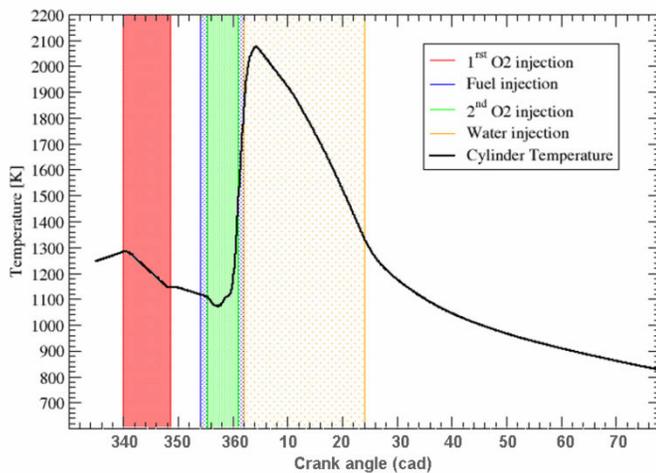
Figure 8: Swirl ratio plot

High cylinder temperature enables the injected fuel to be auto-ignited in the piston bowl. While fuel oxidation is taking place, second delivery of oxygen into the piston bowl replenishes the diminishing oxygen in the bowl. The second oxygen injection is also expected to displace the buildup of carbon dioxide and water from the earlier fuel oxidation. Ensuring adequate supply of oxygen in the piston bowl is crucial to avoid formations of HC, CO and soot.

The second oxygen injection increases the swirl ratio from 14 to more than 15.5. Ensuring high continuous swirl ratio is important as it minimizes the formation of hot spots from the oxygen combustion in the piston bowl. Furthermore, the prolonged high swirl ratio will later assist the distribution of the injected water inside the combustion chamber.



**Figure 9: Fuel Oxidation Profile**



**Figure 10: Cylinder Temperature Plot**

Figure 9 shows very rapid fuel oxidation. Combination of very rapid heat release and low charge mass in the absence of nitrogen is likely to be the reason behind the rapid cylinder temperature increase as shown in Figure 10. In preventing overheating that can be destructive to

engine components, some form of in-cylinder cooling is required. Delivering water at the 50% mass fraction burned (MFB) point cools off the charge without severely affecting the flame development.

Without the water injection, the peak cylinder temperature goes up as high as 2800K and can be even more if more fuel is involved. With direct water injection, the peak cylinder temperature is controlled to around 2100K. The amount of water to be injected depends a lot on the peak cylinder temperature to be achieved. Further fine tuning can be made by varying the water injection timing and water temperature. As a rule of thumb, the exhaust temperature before the EVO point must not be less than 800K. This is to avoid water condensation from the exhaust gas that may wet the cylinder bore surface during the blowdown phase. Low charge temperature at BDC may also cause misfiring in the next firing cycle.

Cylinder pressure at the time of water injection is about 35 bar. At this pressure, the boiling temperature of water drops from 342° to 242° Celsius [20]. As discussed earlier, with water temperature of 320° Celsius at the point of injection, it is likely that significant portion of the water boils almost immediately once it leaves the injector nozzle.

The remaining water that has not vaporized yet is likely to absorb the combustion heat further. This is followed by additional heat absorbed when the water changes phase from liquid to vapor. Even when the injected water is already in vapor form, the heat transfer continues until temperature equilibrium is reached. High specific heat capacities of water in both liquid and vapor states ensure maximum heat absorption at much lower charge mass.

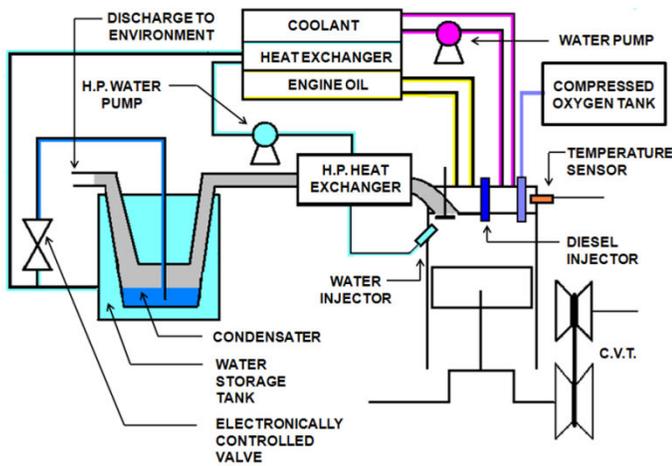
As the water changes phase from liquid to vapor, the cylinder pressure increases rapidly causing the piston to be pushed downward. Steam, having a much higher gas constant  $R$  expands higher than both nitrogen and carbon dioxide gases. This enhances the gas expansion during the expansion stroke.

## OVERALL ENGINE CONCEPT

As shown in Figure 11, a composite tank is used to store oxygen at around 200 bar. Considering that the density of oxygen is much higher than methane's density, relatively higher mass of oxygen can be stored in a typical natural gas vehicle's (NGV) composite tank. With the currently available composite tank technology used for hydrogen storage, it is possible to increase the cylinder pressure to more than 200 bar to store even more oxygen if there is a need to.

Methanol is the preferred fuel if compared to diesel or gasoline. Methanol which is an oxygenated fuel has one of the highest content of oxygen if compared to other oxygenated fuels. With the use of methanol, the oxygen-to-fuel ratio for optimal combustion is less than 1.8:1. This lowers the amount of compressed oxygen to be

carried by the vehicle. This also ensures greater traveling distance between a combined oxygen, water and fuel refilling.



**Figure 11: Overall Engine Concept**

The use of methanol is part of the bigger picture to address the issue of energy sustainability and global warming. Methanol which can be produced from carbon dioxide using the “integrated power and fuel generation plant” [34] provides supply of sulfur free fuel without the need for fuel processing refinery and crude oil supply. The plant which depends on renewable energy sources from sunlight and palm oil derived biofuels for electricity and methanol generations may provide attractive energy solutions in the future [34].

At 200 bar, oxygen can be injected using the oxygen injector without using gas compressor. Furthermore, maximum oxygen injection flow rate is possible, independent of engine speed and load. As the oxygen generation, compression and cooling are done separately at the fuel refilling station, intercooler for cooling the charge is not needed onboard the vehicle.

Heat from the exhaust gas is first transferred to the high pressure heat exchanger while majority of the remaining heat is transferred to the water at the fresh water storage tank which also functions as a condenser. Earlier work by Letsz et al cools off the exhaust gas to a temperature as low as 37.8° Celsius in order to maximize the water reclaim [18]. For this novel cycle, the exhaust gas temperature is reduced to slightly higher charge temperature of 40-50° Celsius. This is to allow the water to be refilled with fresh water regularly at the same time fuel and oxygen tanks are being refilled. Electronically controlled valve regulates the amount of water to be reused.

In-cylinder water injection system in large engine industry has entered serial production with no reported engine components deterioration even after more than 6000 hours of operation [35]. To avoid metal corrosion of engine parts in contact with the injected water, de-

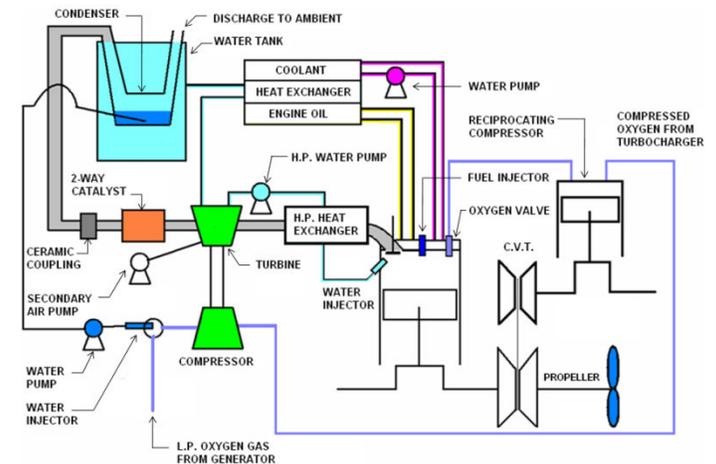
ionized water and corrosion inhibitor are necessary [16]. Fine water filtration is also necessary to prevent impurities from clogging the heat exchangers and water injector. This filtration is also necessary to control impurities above certain size from entering the combustion chamber.

From the water storage tank, the water is then directed to the next heat exchanger where secondary heat from engine oil and coolant is transferred to the water. High pressure water pump increases the water pressure to 150 bar to increase the boiling temperature and specific heat capacity before the heated water enters the high pressure heat exchanger.

Depending on the engine out emissions, 2-way catalyst may be needed to treat HC and CO emissions. This catalyst is sandwiched in between the exhaust port and the high pressure heat exchanger. With no NOx to worry about, equivalence ratio of 0.8 to 0.9 can be used to increase the 2-way catalyst efficiency. This can be done by injecting more oxygen upstream. Another option involves the use of secondary air injection downstream in which regular air can be used instead of high purity oxygen. Operating the engine at slightly lean condition upstream is also expected to improve the engine out emissions.

To minimize heat from being wasted to the environment, all the pipes, heat exchangers, catalytic converter, pumps, valves, tanks, etc. in the system must be very well insulated. The extensive insulation also plays an important role in making sure that the water in the circuit does not freeze in extreme cold temperature.

Air movement in the engine compartment in a moving vehicle must also be minimized to prevent heat losses. This requires the vehicle’s body panel to properly enclose the engine compartment and exhaust system. The vehicle fitted with this novel engine is expected to have low drag as openings for cooling and radiator are no longer required.



**Figure 12: Large engine application**

As shown in Figure 12, with some design revision, the novel cycle is also applicable to large engine covering large mining trucks and marine vessels. Space availability adjacent to the engine enables a dedicated oxygen generator to be used instead of storing the oxygen in a composite tank. Oxygen will later be compressed twice up to around 25 bar, once using a turbocharger and another one using a piston compressor. Water is used to cool off the charge during the gas compression. Heat buildup at the turbocharger is also scrubbed for reuse in the combustion chamber.

With feed pressure as low as 25 bar, the oxygen injector may no longer be suitable thus a revised poppet valve that enables oxygen to be delivered directly into the piston bowl is required. Such revised poppet valve is also currently being developed and technical information about it is not yet available to the public.

**THE USE OF LOW GRADE FUELS** – For marine vessel, the use of high purity oxygen enables residual fuel oil to be used with minimum emissions penalty. Earlier work has confirmed that just by enriching the oxygen content in the air from 21% to 30%, residual fuel oil can be burned with cleaner engine out emissions [36]. Higher oxygen purity at 90-95% when combined with the stratification of oxygen and fuel should yield even better results.

Nevertheless, the large amount of sulfur content in both residual fuel oil and crude oil normally cause high amount of sulfur oxides to be present in the exhaust gas. This requires the sulfur oxides to be dissolved by condensing the water in the exhaust gas. Earlier work by Letsz et al has reported positive result in scrubbing sulfur oxides from the exhaust gas [18]. With significantly higher water-to-fuel ratio used in this novel cycle, the amount of sulfur oxides that can be recovered should also be higher. Upon successful water condensation, the resulting sulfuric acid must be neutralized using alkali injected to the water supply. Any impurities from the reaction must later be filtered.

NO<sub>x</sub> is likely to exist in the exhaust gas because the fuel used may contain some nitrogen percentage. The nitrogen molecules are likely to be liberated during combustion in which the molecules may be oxidized at a later stage. To overcome the excessive NO<sub>x</sub> formation, water injection point can be advanced earlier than the 50% MFR point. The water injection flow rate must also be increased to maximize the presence of water in the cylinder as early as possible. The cooling effect due to large amount of water in the cylinder may reduce the peak cylinder temperature and localized charge temperature to below 2000K point. In addition to that, the equivalence ratio is preferably kept as close as possible to 1.

## IMPROVEMENT IN ENGINE EFFICIENCY

From the perspective of the revised heat engine model, it is desirable to release as much heat as possible to the expander while minimizing heat wasted to the surroundings. Knowing that energy cannot be created or destroyed, the thermal energy in the system is mostly turned into kinetic energy when the piston is pushed downward. As a result, higher useful work can be expected from the system.

Contrary to other engines equipped with heat recovery system, major emphasis is made in minimizing waste heat generation upstream during the combustion and gas expansion. This is expected to yield greater impact in thermal efficiency improvement. Nevertheless, the reduced waste heat is still recovered downstream for reuse.

As discussed earlier, by the time exhaust gas is discharged to the surrounding, the temperature has already dropped to around 40-50° Celsius, indicating that very little energy is lost to the environment through the exhaust gas. A representative from BMW has claimed that it is possible to convert as much as 80% of the heat energy in the exhaust gas into usable power [37]. This article suggested that the required energy conversion technology is already available.

With no coolant or oil radiator required, the engine heat carried out by oil and coolant has to be scrubbed by water and reintroduced into the engine. Assuming that the engine and its related components are very well insulated, large amount of heat is made available to the expander and yet very little heat is wasted to the environment.

In making sure that the useful work can be maximized, it is worth to investigate further from the point of view of enthalpy. A comparison is made between the novel combustion cycle and a combined (or mixed) cycle. A combined cycle involves the use of a primary heat engine and a smaller auxiliary heat engine. An auxiliary turbine or piston engine is used to extract work from the recovered secondary heat.

Assuming that both cycles recover the secondary engine heat well resulting in water to be heated up to the temperature of 320° Celsius and pressure of 150 bar. At this water temperature and pressure, the enthalpy of the water is 1518.5 kJ/kg [20]. In a combined cycle, the heated water is directed straight to the auxiliary heat engine where significant work can be extracted from a piston engine or a steam turbine.

In comparison, this novel cycle is specifically designed for the heated water to be injected directly into the engine. Inside the engine, the heated water will be heated up further to 2000K where the cylinder pressure at that particular piston position is about 40 bar. At this particular charge pressure and temperature, the

enthalpy of water is as high as 6586.5 kJ/kg [38]. With enthalpy this high, the enthalpy of the heated water for the novel combustion cycle is about 4 times higher than the enthalpy of the heated water used in the auxiliary heat engine of the combined cycle. With much higher water enthalpy, the potential for the novel combustion cycle to do useful work shall be higher than what is possible with the combined cycle.

Furthermore, with no auxiliary engine involved by the novel cycle, further benefits can be gained because there will be less power transmission losses with a single work output shaft if compared to two. There is also no additional weight penalty and complexity involved in having only one primary engine instead of two separate engines.

### **COMPARISON BETWEEN ENERGY SUPPLIED BY HYDROCARBON FUEL AND ENERGY SUPPLIED BY HEATED WATER**

A barrel of crude has 6100 MJ of chemical energy [39]. In comparison, 9.5 barrels of water at 320° Celsius and 150 bar pressure has about 6100 MJ of thermal energy. In extracting work from a heat engine, useful work can only be extracted when the piston or turbine is moved. With the ultimate aim of moving the piston or turbine to do work, a comparison is made between the two energy sources.

Fuel containing a much higher energy density releases a lot of thermal energy during combustion. With such a high heat release, majority of the heat is often wasted to the environment while only about 1/3 of heat is converted into useful work when the piston or turbine is moved [1]. Furthermore, several energy conversions are involved in the process, the first one involves the conversion from chemical energy to thermal energy and the second one involves the conversion of thermal energy to kinetic energy. The process is also irreversible.

In comparison, heated water at the previously specified temperature and pressure can be used directly to move a small turbine or piston heat engine. Nevertheless, unless the water is further heated up, its energy density and enthalpy is still too small thus the potential to do useful work is limited.

Even though the energy contents of the two are the same, each energy source has its own set of problems that hinders it from realizing its full potential. In solving these two sets of problems, it is proposed through this novel cycle for the two energy sources to be combined to benefit one another.

By injecting the heated water during the intense heat release from fuel oxidation, the amount of heat wasted can be minimized. At the same time, the low energy density and enthalpy of water can be improved once the heated water absorbs the combustion heat.

Effectively the shortcomings of both fuel and heated water are addressed simultaneously by getting these two elements to work together rather than to work independently. Assuming that the expander is a system on its own, about half of the energy is introduced into the expander using hydrocarbon fuel and the other half is introduced using heated water. In theory, the expander can either do more work using the same amount of hydrocarbon fuel or it can do the same amount of work using less hydrocarbon fuel.

Water temperature of 320° Celsius and water pressure of 150 bar are estimated to give a good balance in terms of energy density, water compression power requirement and material limit. Considering that the amount of energy that can be recovered from the engine secondary heat is limited to the actual amount of secondary heat rejected by the engine itself, energy that is recoverable is actually limited. In particular, with higher heat absorption during combustion, relatively lower heat is rejected to the exhaust gas, oil and coolant if compared to the conventional engines. Therefore, it is not likely that the water-to-fuel ratio for water injection to exceed 9.5:1.

As shown in Figure 2, there is an option to obtain thermal energy from external sources like sunlight, geothermal, mechanical friction, brake system, industrial waste heat, etc. The option to obtain heat from external sources is highly desirable because low grade heats are abundantly and easily available. Any heat source that has temperature higher than the water temperature itself can be used as an external heat source. By flowing water at room temperature over multiple heat sources that are arranged in series, considerable amount of thermal energy can be collected and reused.

Therefore, it is not impossible for the water-to-fuel ratio for water injection to exceed the 9.5:1 ratio. With large amount of heat supplied from external sources, it is also not impossible for work output in every cycle to exceed the chemical energy supplied by the fuel in every cycle.

### **CONCLUSION**

The use of stratified fuel and oxygen enables rapid availability of intense heat that is crucial for combustion cycle with water injection. Combustion efficiency is also improved, which in turn lowers HC, CO and PM engine out emissions. Lack of nitrogen during combustion on the other hand minimizes formation of NOx. When combined with a novel exhaust valve timing and lift strategy, multi fuel operation is possible enabling a broader range of fuels to be used using the same engine.

Innovative water injection system enables water to be delivered into the combustion chamber without significantly affecting the flame development. This enables water to replace air as the working medium. Water as a working medium unlocks so many

possibilities that are beneficial for energy conservation and environment.

Water which can exist in both liquid and vapor forms can be manipulated to exist in either liquid or vapor by changing its pressure and temperature. This enables water in liquid form to be used to scrub heat and to transport the scrubbed heat into the combustion chamber. Once inside the combustion chamber, the heated water will absorb the combustion heat and be turned into vapor. Once in vapor state, it will enhance the gas expansion during the expansion stroke.

From the study, it is also discovered that heated water when combined with fuel oxidation compliments one another, resulting in higher work output. Furthermore, by using water to transport heat from low grade heat sources into the heat engine, reliance of heat engines on fossil fuels may be reduced from time to time. With much lesser fuel consumed by heat engines to generate the same amount of power, renewable fuels that are currently costly to use at the moment may become cost effective in the future.

The research is yet to enter the physical testing stage. Nevertheless, theoretical evidences and preliminary simulation results discussed in this paper have suggested that the novel cycle has a good potential to achieve higher theoretical efficiency if compared to the existing Diesel and Otto cycle. The author is hopeful that the information presented in paper is sufficient to generate interests among the researches around the world to conduct deeper research in this relatively new area of engine technology. With more involvements from others, there should be more dedicated software and engine parts which are currently lacking to support the research.

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