Numerical investigation of CAI Combustion in the Opposed-Piston Engine with Direct and Indirect Water Injection

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Abstract. This paper is focused on the CAI combustion control in a turbocharged 2-stroke Opposed-Piston (OP) engine. The barrel type OP engine arrangement is of particular interest for the authors because of its robust design, high mechanical efficiency and relatively easy incorporation of a Variable Compression Ratio (VCR). The other advantage of such design is that combustion chamber is formed between two moving pistons – there is no additional cylinder head to be cooled which directly results in an increased thermal efficiency. Furthermore, engine operation in a Controlled Auto-Ignition (CAI) mode at high compression ratios (CR) raises a possibility of reaching even higher efficiencies and very low emissions. In order to control CAI combustion such measures as VCR and water injection were considered for indirect ignition timing control. Numerical simulations of the scavenging and combustion processes were performed with the 3D CFD multipurpose AVL Fire solver. Numerous cases were calculated with different engine compression ratios and different amounts of directly and indirectly injected water. The influence of the VCR and water injection on the ignition timing and engine performance was determined and their application in the real engine was discussed.

1. Introduction
The possibility of achieving high thermal efficiency brings Opposed-Piston (OP) engines back into interest of research centers. An advantage of such design is that combustion chamber is formed between moving pistons. The main thermal benefits arise from the geometrical shape of the combustion chamber. As heat loses are proportional to the area $A$ of the reactor and heat generation is proportional to the volume $V$, the factor $A/V$ is simple but very efficient estimator of internal combustion engine efficiency and in OP engines it is twice lower than in conventional SI [1]. In the OP engine designed as a 2-stroke the poppet valves become redundant and with adapting an uniflow scavenging, the volumetric, trapping and scavenging efficiency become comparable with a 4-stroke. Because of the lack of the cylinder head, a scavenging process need to be handled differently than in a conventional 4-stroke engine. In the OP engine usually intake and exhaust ports in the cylinder liner are responsible for the scavenging. When pistons reach their Bottom Dead Centre (BDC), ports are opened and charge is exchanged due to pressure difference between the intake and exhaust manifolds.

There are several types of OP engine configurations (crankless, single crankshaft, multiple crankshaft, rotary or barrel) [2]. The barrel type OP engine is of particular interest for the authors because of its robust design, high mechanical efficiency and relatively easy incorporation of a Variable Compression Ratio (VCR) [3]. In the barrel type OP engine cylinders’ axes are parallel to the drive shaft axis. Linear to rotary motion is changed through the special plate with connecting rods mounted on ball bearings. An 8-cylinder barrel type OP piston engine concept is presented in Błąd! Nie można odnaleźć źródeła odwołania.
Another measure for increasing engines efficiency is Homogeneous Charge Compression Ignition (HCCI)/Controlled Auto-Ignition (CAI) combustion mode. It is an unique form of combustion based on charge auto-ignition at desired crank angle. It has been demonstrated that a CAI gasoline engine can achieve fuel economy levels comparable to those of a Compression Ignition (CI) engines, while producing engine-out NOx emissions that are as low as tail-pipe NOx emissions from a conventional SI engine equipped with a three-way catalyst [4]. Although the idea of HCCI/CAI combustion is desirable, it is also very challenging to implement in an internal combustion engine due to the absence of direct ignition timing control (i.e. spark). In order to guarantee correct combustion timing, closed-loop combustion control is necessary. This type of control is supposed to vicariously influence the ignition timing via different measures (i.e. VCR or water injection).

This paper is focused on the CAI combustion control in a turbocharged 2-stroke barrel-type opposed-piston engine which is currently under development at Warsaw University of Technology. The engine will be equipped with an online VCR and water injection for indirect ignition timing control. The water injection is also supposed to prevent knock by charge cooling through evaporation and extend engine operation area. Water will be injected either directly into the cylinder or indirectly into the intake manifold. The turbocharging will increase the engine power output. Such a complex CAI combustion control system is challenging to implement in the real engine. Therefore, numerical simulations can become a useful tool for better understanding of the combustion process and can shorten the time span for engine development. In this study 3D CFD numerical simulations of the scavenging, injection and combustion processes were performed in order to determine possible engine operating points in CAI combustion mode.

2. HCCI/CAI fundamentals and modeling

In a conventional SI engine combustion starts when an electrical spark is used to initiate a flame kernel that develops across the combustion chamber in a turbulent manner. During HCCI/CAI combustion auto-ignition takes place when the conditions are right in terms of temperature and pressure for the particular mixture of fuel and air. However, the type of ignition and further combustion differ between HCCI and CAI leading to different benefits of these two types of combustion and different strategies of the ignition and combustion control. In the HCCI mode premixed, homogeneous mixture ignites at multiple sites and invokes the simultaneous reactive envelopment of the entire fuel/air mixture without a flame front. The heat release process is much faster than the conventional SI combustion and is most likely to result in undesired knock. In order to limit the heat release rate and prevent knock HCCI engines usually work with charge highly diluted either by the excess of air or by EGR. In cases where charge stratification occurs, the mixture will ignite at a single spot, where it firstly reach the ignition condition and the flame will propagate across the combustion chamber. Although this Controlled Auto-Ignition (CAI) operation is similar to conventional SI combustion, the conditions (pressure and temperature) in the chamber at the moment of ignition would lead to undesired knock in case of stoichiometric mixture. Hence, engines in CAI mode, similarly as in HCCI mode, work with lean mixtures.

In recent years various experimental and numerical studies of HCCI/CAI combustion have been carried out [4–8]. Researchers investigated mainly conventional 4-stroke engines proving that with VCR or intake charge heating it is possible to achieve CAI combustion and indirectly control ignition timing.
Engine operation in this mode is usually limited to low and medium loads due to reduced equivalence ratios for avoiding knock. However, with proper internal or external EGR, thermal and fuel stratification even a stoichiometric charge can be combusted with acceptable pressure-rise rates. Furthermore, supercharging is one way to dramatically increase IMEP for HCCI and extend its operation area.

In order to properly predict ignition and combustion in the engine running in CAI/HCCI mode it is necessary to account for the charge stratification and wall interaction, what leads to multi-dimensional CFD modeling. Furthermore, HCCI/CAI ignition of heavy hydrocarbons is a two-stage process involving a low temperature cycle followed by a high temperature cycle [4] so the fuel chemical kinetics plays a dominate role during the whole combustion process. With rapid growth of the HCCI/CAI engine research, the study on chemical kinetics mechanism of different surrogate fuels which can properly describe combustion characteristics in these new concept engines has become very active. The attention was focused on reduced mechanisms which can be applied directly to the engine combustion simulation using multidimensional CFD codes. In recent years several mechanisms were developed for iso-octane which exhibits similar trends to gasoline over the HCCI operating range [9–12]. The most recent one is by Liu et al. [12] and consists of 32 species and 111 reactions. Authors validated their skeletal model against experimental data in various reactors under diverse operating conditions, with emphasis on laminar flame speed and important species evolution. The predicted results showed good agreement with experiments. Also, the performance of the mechanism was compared to that of other reduced mechanisms available in the literature, showing its superiority in a HCCI relevant conditions.

3. Engine setup
This study concerns numerical simulations of CAI combustion in the Opposed-Piston engine being currently under development at Warsaw University of Technology. The investigated research engine is a 2-cylinder, 2-stroke, barrel-type OP engine with cylinders’ axes parallel to the shaft axis. The basic engine parameters are given in Table 1.

| Engine parameters | 2-stroke, OP, turbocharged |
|-------------------|---------------------------|
| Number of cylinders | 2                         |
| Bore              | 0.055 m                   |
| Displacement volume | ~1800 ccm               |
| Engine speed      | 1500 rpm                  |
| Compression ratio | VCR 8±18                  |
| Fuel              | Gasoline                  |
| Ignition          | SI/CAI                    |
| Fuel injection    | Direct Injection (DI)     |
| Water injection   | Direct/Manifold (DWI/MWI) |

The biggest challenges associated with CAI combustion are ignition timing control and operation outside the knock area. As for the knock, it is usually related to excessive heat release rate and can be avoided in CAI engines running with reduced equivalence ratios. However, it is desirable to reduce heat release rate with different methods in order to increase equivalence ratio and extend the engine operation area to higher loads. The investigated engine will be equipped with the following solutions that will allow CAI combustion control:

- Variable Compression Ratio for indirect ignition timing control
- Variable Port Timing for scavenging and EGR control
- Direct fuel injection for fuel stratification and limiting the heat release rate
- Manifold Water Injection for indirect ignition timing control and limiting knock
- Direct Water Injection for ignition control through direct internal EGR cooling
- Turbocharging for increased engines IMEP and wider operation area
4. Simulation setup

4.1. Numerical mesh and boundary conditions
Numerical simulations of combustion in this study were performed using the AVL Fire 3D CFD solver based on Finite Volume Method (FVM) discretization. Firstly, numerical mesh was prepared. Simulations were performed for one cylinder and half of the intake and exhaust manifolds. Two types of meshes were defined – steady mesh for intake/exhaust manifolds and moving mesh for cylinder volume. Movement of the cylinder mesh was handled by changing positions of the nodes representing intake-side and exhaust-side pistons separately according to the given piston displacement curves. Simultaneously, positions of the nodes between pistons were interpolated every time step according to the pistons displacement. Meshes of the cylinder and intake/exhaust manifolds were connected with Arbitrary Interface at the contact of the cylinder wall and intake/exhaust ports. Total number of mesh elements for the entire model was of 1,200,000, while mesh for the cylinder itself consisted of 200,000 elements. The mesh of the cylinder used for simulations together with applied temperature boundary conditions is presented in Figure 2. In this study temperature on the intake side piston wall was assumed to be $T_{\text{in}} = 800\,\text{K}$, temperature on the exhaust side piston $T_{\text{ex}} = 880\,\text{K}$ and on the cylinder wall a temperature distribution was defined in range of $T_c = 400–800\,\text{K}$. Such high temperatures were assumed due to the high engine thermal load.

4.2. Combustion modeling
There are various combustion models available in commercial CFD solvers for premixed or non-premixed combustion. In case of piston engines these models are usually developed for SI and CI combustion [1]. Although combustion models predict Auto-Ignition, they are not be suitable for low temperature combustion of CAI. In order to account for modeling both low and high temperature combustion of transportation fuel surrogates, such as iso-octane it is necessary to use reduced kinetic schemes. In this study one of the most recent reduced mechanisms developed by Liu et al. [12] for iso-octane HCCI/CAI combustion was used. Additionally, a submechanism for NOx formation was taken from [10] and included in the Liu scheme. Final kinetic scheme for iso-octane oxidation used for CAI combustion simulations in this study consisted of 37 species and 124 reactions.

Turbulence is a key issue in CFD modeling of processes taking place in combustion engines. It has to be taken into account in combustion simulations. In this work $k-\zeta-f$ turbulence model was used for turbulence modeling. It is a four-equation model developed by Hanjalic et al. [13] which solves equations for turbulent kinetic energy $k$, turbulent kinetic energy dissipation rate $\epsilon$, normalized velocity scale $\zeta$ and explicit relaxation function $f$. The model details are given in [1] and [13].

4.3. Operating conditions in simulations
In previous sections several solutions for CAI combustion control in 2-stroke OP engine were named and described. In order to limit the number of investigated cases in this study only two measures relevant
for CAI combustion were considered – VCR and water injection. A constant boost pressure of 3 bars (absolute) was assumed for the simulations to increase engine power output. Reduced equivalence ratios were considered to limit the maximum pressure rise and avoid knock. Operating conditions for this study are summarized in Table 2.

Table 2. Engine operating conditions

|                          | 3 bar (absolute) |
|--------------------------|------------------|
| Boost pressure           | 3 bar (absolute) |
| Intake temperature       | 410 K (at 3 bar boost) |
| Equivalence ratio        | 0.4÷1.0          |
| Compression Ratio        | 8÷12             |
| Fuel in simulations      | iso-octane       |
| Fuel direct injection    | 45÷120 mg/cycle  |
| Start of fuel injection  | -120°CA ATDC     |
| Fuel temperature         | 300 K            |
| Water Injection          | 0÷130 mg/cycle   |
| Start of Direct Water Injection | -160°CA ATDC    |
| Water temperature        | 300 K            |

5. Results and discussion

5.1. Operation targets for investigated cases
Simulations were performed for different compression ratios, equivalence ratios and different amounts of directly or indirectly injected water. For each case two engine cycles were calculated. For the first cycle approximate initial conditions in the cylinder before the scavenging were assumed. At the end of the first cycle realistic conditions in the cylinder were obtained for the second cycle scavenging and combustion. Only results from the second cycle are presented and compared in this study.

In order to compare the results and draw conclusions specific targets for the combustion results need to be assumed. In this study following parameters are considered:

- Crank angle of 50% accumulated heat release (CA50) was considered as a measure of combustion timing [4]. Target for CA50 in this study was ±1.0°CA ATDC
- Maximum pressure rise dP/dCA was assumed as the limiting parameter for the knock, since the knock itself was not modeled in this work. Target for maximum dP/dCA was of 20 bar/CA

In CAI combustion high temperature heat release is followed by the low temperature heat release. Low temperature combustion usually starts earlier in the cycle and is responsible for 5% to 10% of the total heat released depending on the fuel [4]. For the iso-octane reduced scheme used in this study low temperature combustion delivers ~5% of the total heat released. The crank angle at which 5% of the heat is released (CA5) can be considered as the high temperature ignition. However, in this study CA5 timing was not analyzed and focus was paid only on the CA50 timing adjustment.

5.2. CAI without water injection
Firstly, engine operation in CAI mode without water injection was investigated. In order to meet the targets for CA50 and dP/dCA it was necessary to work with the lowest possible compression ratio of CR=8. Results for this operating point are given in Figure 3.
Clearly, the engine cannot work with stoichiometric mixture under these conditions due to excessive heat release resulting in high maximum pressure rise and probably knock. Hence, equivalence ratio need to be lowered to the level of $\phi=0.5$ at which $dP/d\text{CA}=20.9 \, \text{bar/CA}$ and $\text{CA}50=0.3^\circ \text{CA ATDC}$. It can be seen that $\text{CA}50$ timing differs with the equivalence ratio significantly. It is due to different combustion duration. On the other hand $\text{CA}5$ timing differs with the equivalence ratio only slightly meaning that equivalence ratio has small impact on the high temperature ignition timing of the mixture.

In order to have a benchmark for CAI combustion performance, an additional case of conventional SI combustion with indirect gasoline injection (intake manifold injection MI) in the investigated engine was calculated for compression ratio of $\text{CR}=9$ and equivalence ratio of $\phi=1.0$. To make the case comparable with the CAI cases, the boost pressure and intake temperature were adjusted for similar power output. Also ignition timing was adjusted for $\text{CA}50$ to occur at TDC.

![Figure 3. Results of pressure trace, ROHR, CA50 and CA5 for CR=8.](image)

5.3. CAI with water injection

The possibility of adjusting compression ratio is of particular importance for CAI combustion control. Raising the compression ratio is expected to result in an increased engine efficiency and lower fuel consumption. In previous section CAI combustion was obtained for the fixed compression ratio of $\text{CR}=8$. If one would increase the compression ratio, simultaneously auto-ignition would occur too early and affect the engine operation. The other solution for indirect ignition control proposed by the authors is water injection. The water injected into the intake manifold would cool the intake charge through the evaporation and retard the ignition. Additionally, it could increase the charge thermal stratification and limit maximum heat release and knock. The water can be also injected directly into the cylinder during the scavenging process. In that case evaporation takes place inside the cylinder and have more direct impact on the cylinder walls but can result in uneven water distribution.

In order to investigate simultaneous application of the VCR and water injection in CAI engine a number of cases was calculated including compression ratios of $\text{CR}=8, 9, 10, 11$ and $12$. Considered amount of injected water was ranging in $0\div130 \, \text{mg/cycle}$. In case of Manifold Water Injection (MWI)
water evaporation calculations were carried out separately and their results were applied as initial conditions in the intake manifold for CFD simulations. For Direct Water Injection (DWI) water was injected into the cylinder with a pintle-type injector during the scavenging process. The injection timing should be as early as possible for droplets to have more time for evaporation. On the other hand injection should not be too early in order for water not to reach the exhaust. The best timing for the start of DWI in investigated cases was determined to be -160°CA ATDC.

Results of the temperature field at the cross-section of the cylinder and water droplets for different amount of the injected water just after the intake ports closing are compared in Figure 4. Thermal stratification developed during the scavenging is clearly visible. Differences between Direct and Manifold Water Injection are also visible. In case of MWI and 30 mg/cycle of water all droplets evaporated before the end of the scavenging. For 60, 90 and 120 mg/cycle intake temperature was too low for all droplets to evaporate. Droplets which entered the cylinder are distributed in the whole volume and are slightly more concentrated on the intake side. Their evaporation during the compression stroke increases the thermal stratification. High temperatures remains at the exhaust side of the combustion chamber. The Direct Water Injection behavior is different. During the injection water droplets are drifted by the scavenging air momentum to the exhaust side of the cylinder. The internal EGR and exhaust side piston are cooled by the injected water, while intake side of the cylinder remains unaffected, what means that thermal stratification is reduced. Direct Water Injection might be effective in ignition timing control. However, its influence on the heat release rate and knock is expected to be limited because of the uneven water distribution in the cylinder.

![Figure 4](image)

**Figure 4.** Temperature fields and water droplets after the scavenging at -120°CA ATDC. Manifold Water Injection on the left and Direct Water Injection on the right

| Case       | Combustion mode | Equivalence ratio [-] | Absolute boost pressure [bar] | Fuel mass [mg] | Water mass [mg] | Water to Fuel ratio | dP/dCA [bar/CA] | CA50 [CA] | EGR [-] |
|------------|-----------------|-----------------------|--------------------------------|----------------|----------------|---------------------|-----------------|------------|---------|
| CR9 SI     | SI              | 1.0                   | 1.2                            | 61.7           | -              | -                   | 15.8           | 0.4        | 5.5%    |
| CR8 CAI    | CAI             | 0.5                   | 3.0                            | 58.5           | -              | -                   | 20.6           | 0.3        | 5.1%    |
| CR9 DWI    | CAI with        | 0.4                   | 3.0                            | 46.8           | 5              | 0.10                | 18.8           | -1.1       | 5.5%    |
| CR10 DWI   |                 | 0.45                  | 3.0                            | 48.5           | 70             | 1.44                | 16.7           | 0.5        | 10.6%   |
Equivalence ratio adjustment for higher compression ratios with water injection was performed similarly as for CR=8 in section 5.2. Of course, combination of compression ratio and water injection required calculating considerable number of cases. Firstly, cases with equivalence ratio of $\phi=0.5$ were calculated in order to determine which combination of the VCR and water injection is the closest to defined limits. Then, final adjustments were done to fit the targets. Finally defined operating points for each investigated compression ratio are given in Table 3 together with the benchmark SI combustion case. It is interesting to compare Direct and Manifold Water Injection for the same compression ratios. For CR=9 only 5 mg/cycle of DWI was enough to meet the CA50 target. However, water injection cooled down only the surroundings of the exhaust piston wall and it was necessary to lower the equivalence ratio to the $\phi=0.4$ to fit the dP/dCA limit. On the other hand MWI of 30 mg/cycle for CR=9 helped to meet the CA50 target, but the water was evenly distributed and it was possible to maintain equivalence ratio of $\phi=0.5$ for the dP/dCA limit. For the higher compression ratios the trend was different and more water needed to be injected directly than into the manifold to obtain defined targets. It can be explained by the fact that DWI had more impact on the exhaust side of the cylinder volume and was less effective in cooling down the intake side of the cylinder volume, while for the MWI water was more evenly distributed in the whole cylinder volume.

5.4. Ignition positioning

Water injection for CAI combustion influence not only ignition timing, but also ignition positioning. The charge will ignite at the position where ignition conditions are firstly achieved. Probably wall temperatures are of importance for ignition in CAI combustion mode. Results of ignition positioning together with remaining water droplets are given for final cases in Figure 5.

![Figure 5](https://example.com/image.png)

**Figure 5.** Ignition positioning in investigated cases. Exhaust-side piston in the front, intake-side piston in the back.

In case of SI combustion spark ignition at the cylinder wall is visible. For CAI combustion with Manifold Water Injection ignition always occurred at the exhaust-side piston wall. It was because of the high wall temperature and surrounding of the high-temperature internal EGR. Remaining water droplets
are visible for higher compression ratios, for which more water was injected. As for Direct Water Injection, it is visible that the water was dragged to the exhaust-side piston and most of it evaporated in this area during the compression stroke. In the effect surroundings of the exhaust-side piston were cooled down, so that the ignition relocated to the cylinder wall for CR10 DWI, CR11 DWI and CR12 DWI cases. More water droplets remain unevaporated than in MWI cases due to less time available for evaporation and increased water concentration at the exhaust-side of the chamber.

These results suggest that it might be beneficial to simultaneously inject water directly into the cylinder and indirectly into the intake manifold in order to retard the ignition even more for higher compression ratios. Water injected into the manifold would be more efficient in cooling down the intake-side piston and intake-side of the cylinder volume, while water injected into the cylinder would directly affect exhaust-side piston as well as high temperature EGR and its surroundings.

5.5. Performance and emissions for final operating points

In order to determine what was the effect of an increased compression ratio and water injection on the engine performance such parameters as IMEP, indicated efficiency and emissions are compared for the final operating points from Table 3 and presented in Figure 6. If it comes to IMEP (which also corresponds to engine power output), it is related to the engines load and cannot be directly compared between different compression ratios. However, it can be seen that generally with Manifold Water Injection IMEP was increased. It was due to lower intake temperatures, which allowed to trap more air in the cylinder, as well as maintain equivalence ratio at the level of $\phi=0.5$. On the other hand, Direct Water Injection decreased IMEP, because of the worse scavenging (more EGR trapped in the cylinder). Additionally, for CR9 and CR10 cases equivalence ratio needed to be adjusted for dP/dCA limit, which also contributed to the lower power output. The lowest results were obtained for CR9 case with Direct Water Injection, while the highest results were for CR12 case and Manifold Water Injection.

![Figure 6](image)

**Figure 6.** IMEP, indicated efficiency, CO and NOx emission

The engines efficiency is probably of more importance than power output, because it directly translates into the specific fuel consumption. Performed simulations prove that switching from SI mode to CAI mode results in efficiency increase. Then, in CAI mode with Manifold Water Injection efficiency was further increased with the compression ratio reaching 46.1% for CR=12. Although this trend is not
clear with Direct Water Injection, for this mode the efficiency was generally higher for higher compression ratios. Differences between cases with DWI might be related to uneven water distribution that affected heat transfer coefficient and heat losses to the cylinder wall. Finally, the maximum efficiency of 46.1% obtained for CAI combustion is a significant improvement in regard to the benchmark SI combustion efficiency of 38.4%.

The most important result nowadays are emissions. For considered operation points switching from SI to CAI combustion decreased the NOx emission by over 20%. It was mainly due to lower equivalence ratio which resulted in lower maximum local temperatures. As for the CAI with Manifold Water Injection NOx emission was also decreased with every compression ratio increase. The more water was injected, the lower maximum local temperatures and local oxygen concentrations were, what favored decrease in NOx formation. In case of Direct Water Injection NOx reduction was even more effective for compression ratios CR=9 and CR=10. However, it was caused mainly by the reduced equivalence ratio in these two cases. For CR=11 MWI was more effective in NOx reduction than DWI, while for CR=12 similar, very low NOx emissions were obtained for MWI and DWI.

When it comes to CO emission, switching from stoichiometric SI combustion to CAI mode resulted in significant CO concentration reduction in exhaust gases. It was possible due to air excess which allowed for CO to CO$_2$ oxidation at temperatures above 1500 K. CO emission remained low for CR9 and CR10 cases (despite the water injection method). With more water injected in CR11 and CR12 cases CO emission was increased probably due to lower combustion temperatures that inhibited CO oxidation. CR10 and CR11 cases can be considered as a trade-off between CO and NOx emission.

6. Conclusions
In this study CAI combustion in a 2-stroke barrel type OP engine with direct gasoline injection was investigated. The VCR and water injection were considered for the ignition timing control. 3D CFD numerical simulations were performed in conjunction with a reduced kinetic scheme for iso-octane oxidation in order to account for both low and high temperature heat release. To avoid excessive heat release and knock in case of CAI combustion equivalence ratio was adjusted to the level of $\phi=0.4-0.5$ for investigated cases. Possible CAI engine operating points were determined and performance results were compared with conventional SI engine operation. Simulations proved that with VCR and water injection it may be possible to indirectly control the ignition timing in the OP engine working in CAI combustion mode. Furthermore, in defined operating points engine efficiency was improved in CAI mode. As for emissions, NOx concentration in exhaust gases was significantly reduced with water injection thanks to lowered combustion temperatures while CO emission can also be reduced with CAI mode as long as temperatures after the combustion process are sufficient for CO to CO$_2$ oxidation.

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