# Reduction in $NO_x$ and CO Emissions in Stoichiometric Diesel Combustion Using a Three-Way Catalyst

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*Experimental and numerical studies were performed to investigate the simultaneous reduction in $NO_x$ and CO for stoichiometric diesel combustion with a three-way catalyst. A single-cylinder engine was used for the experiments and KIVA simulations were used in order to characterize the combustion efficiency and emissions of throttled stoichiometric diesel combustion at 0.7 bar boost pressure and 90 MPa injection pressure. In addition, the efficiency of emission conversion with three-way catalysts in stoichiometric diesel combustion was investigated experimentally. The results showed CO and $NO_x$ emissions can be controlled with the three-way catalyst in spite of the fact that CO increases more at high equivalence ratios compared with conventional diesel combustion (i.e., lean combustion). At a stoichiometric operation, the three-way catalyst reduced CO and $NO_x$ emissions by up to 95%, which achieves lower emissions compared with conventional diesel combustion or low temperature diesel combustion, while keeping better fuel consumption than a comparable gasoline engine.* [DOI: 10.1115/1.4000290]

*Keywords: group-hole nozzles, GHN, stoichiometric diesel combustion, fuel economy, $NO_x$ emission reduction*

## 1 Introduction

For decades many new combustion regimes have been suggested to meet stringent emission standards for diesel engines. For example, homogeneous charge compression ignition (HCCI) diesel combustion has been proposed to reduce $NO_x$ and soot emissions, which come from locally high temperature or rich-mixture areas in the cylinder [1–4]. However, in order to be adopted in commercial diesel engines, obstacles like producing the homogeneous charge without spray wall-wetting and combustion phasing control still exist. Other proposed advanced combustion concepts (e.g., low temperature combustion (LTC) and modulated kinetics (MKs) combustion) also have technical issues to be solved [5–8], such as controlling pressure rise rates and high CO and hydrocarbon (HC) emissions.

The other way to reduce diesel emissions effectively is to use aftertreatment. It is known that soot emissions are manageable by introducing a diesel particulate filter (DPF) [9,10]. However, $NO_x$ control using aftertreatment is still an issue because conventional diesel engines operate at low equivalence ratios. This makes it difficult to convert $NO_x$ to nitrogen due to the lack of a reductant like CO or HC, which leads to the need to introduce additives. Selective catalytic reduction (SCR), one of the most promising aftertreatment approaches for diesel $NO_x$ reduction, requires the use of urea as a reductant source, and this requires a suitable infrastructure for wide-spread use. Lean $NO_x$ trap (LNT) technology also sacrifices fuel efficiency [11], and it is still under development.

Lee et al. [12,13] suggested the concept of stoichiometric diesel combustion to allow the use of a three-way catalyst (TWC), as in gasoline engines to control $NO_x$ emissions. This technology has attracted attention because it does not require any reductants. In addition, the technology of the three-way catalyst has been well developed for gasoline engines and it also has benefits in costs compared with SCR or LNT. Previous studies by Lee and Reitz [12,13] focused on increasing exhaust gas recirculation (EGR) to achieve stoichiometric combustion for the operation of a three-way catalyst. They reported that stoichiometric diesel combustion led to around 7% sacrifice in fuel consumption, mainly due to high CO and HC in the exhaust. In order to enhance the fuel consumption in stoichiometric diesel combustion, Park and Reitz investigated new injector nozzle concepts including group-hole nozzles [14] and two-spray-angle, group-hole nozzles [15], and found that the utilization of oxygen can be increased significantly compared with conventional nozzles.

Chase et al. [16] achieved stoichiometric combustion using throttled-intake pressure instead of introducing high EGR to avoid excessive particulate matter (PM). They showed that the PM can be reduced to a manageable level by a DPF.

In the present study, the combustion and emission characteristics of throttled stoichiometric diesel combustion have been investigated experimentally and numerically. In addition, the possibility of reduction in emissions (CO, $NO_x$, and HC) using a three-way catalyst is shown experimentally.

## 2 Experimental Setup

The experimental engine used in the present study was a single-cylinder, direct-injection diesel engine based on a GM 1.9-l, four-cylinder double overhead camshaft (DOHC) engine. The engine's swirl ratio can be adjusted by two swirl control butterfly valves in the intake ports. The engine specifications are listed in Table 1.

A schematic diagram of the experimental apparatus is illustrated in Fig. 1. A TWC of 0.75 l capacity developed for a four-cylinder 2.0 l gasoline-powered vehicle was installed in the exhaust line. An electric heater in front of the TWC was employed in order to compensate for heat loss through the exhaust surge tank and exhaust line. Gaseous emissions were measured before and after the electric heater in order to assure that the heater does not affect exhaust gas concentrations. In the present 0.7 bar

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Table 1 Engine specifications

| | |
|---|---|
| Engine type | Single cylinder direct-injection |
| Bore (mm) | 82 |
| Stroke (mm) | 90.4 |
| Compression ratio | 15.5 |
| Displacement ($cm^3$) | 477 |
| Piston geometry | Open-crater-bowl |
| Intake ports | 1 helical and 1 tangential |
| Swirl ratio | 2.2–5.6 |
| Bowl diameter (mm) | 49.4 |
| Intake valve opening (IVO) (ATDC) | 344 |
| Exhaust valve closing (IVC) (ATDC) | −132 |
| Exhaust valve opening (EVO) (ATDC) | 112 |
| Exhaust valve closing (EVC) (ATDC) | 388 |

Table 2 Engine operating conditions

| | |
|---|---|
| Intake pressure | 0.70 bar |
| Exhaust pressure | ~1.0 bar |
| Intake temperature | 80°C |
| EGR | 0% |
| Swirl ratio | 2.2 |
| Fuel rate | ~19 mg/cycle |
| Injection pressure | 90 MPa |
| SOI | 16–8 before top dead center (BTDC) |
| Equivalence ratio | 1.0 |
| Nozzle hole diameter | 128 $\mu$m |
| Number of holes | 8 |
| Included angle | 130 deg |

"throttled" intake experiments, the external EGR line was completely closed and the intake pressure was set to be around 0.7 bar to achieve the stoichiometric operating condition with approximately 19 mg/cycle fueling. Three different equivalence ratio measurements based on air and fuel flow rates, carbon balance, oxygen balance, and exhaust lambda sensor readings were closely monitored during the engine experiments in order to assure stoichiometric conditions. −8 deg after top dead center (ATDC) injection timing was the latest start-of-injection (SOI) timing allowed under this operating condition [17]. Use of SOI timing after −8 deg ATDC eventually resulted in misfire. It was found that the latest SOI timing was optimal for fuel economy under this "throttled-intake stoichiometric diesel" operation [17]. Details of the engine operating conditions are listed in Table 2. The engine speed was 2000 rpm in all of the experiments.

## 3 Numerical Method

In order to simulate throttled stoichiometric diesel combustion, a multidimensional computational fluid dynamics (CFD) code, a version of the KIVA-3V code [18] with improvements in various spray and chemistry models developed at the Engine Research Center, University of Wisconsin-Madison [19] was used.

Considering that the test engine has an eight-hole fuel injector nozzle, a 45 deg-sector of the combustion chamber was used for the present calculations, as shown in Fig. 2. In order to predict motoring pressure correctly, additional volume was added to the top land crevice area, while keeping the crevice depth identical to the experimental engine.

The ERC-PRF n-heptane mechanism [20], which consists of 39 species and 131 reactions and was reduced from larger detailed mechanisms, was used to achieve manageable computational times. The CHEMKIN chemistry solver was integrated with the KIVA

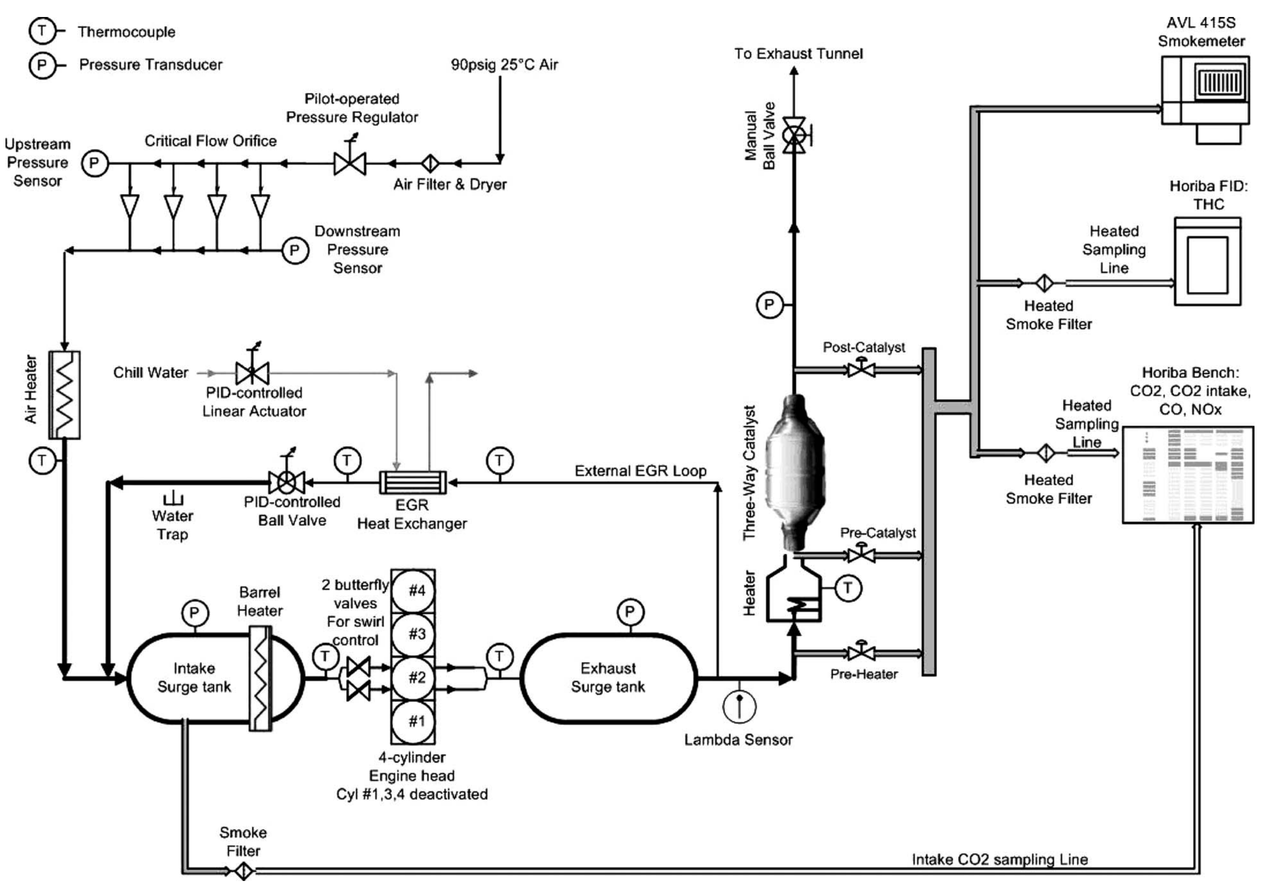


Fig. 1 Schematic diagram of experimental apparatus

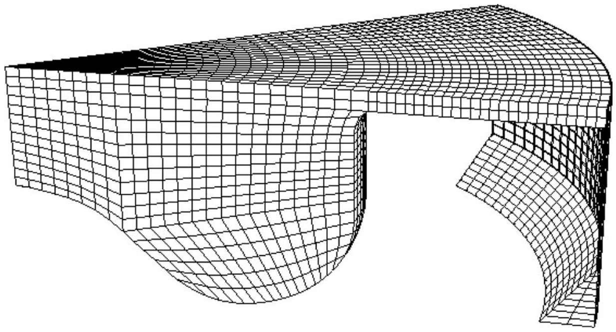

Fig. 2 Computational mesh at TDC

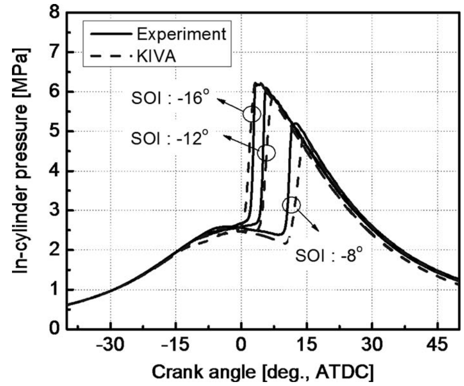


Fig. 3 Model validation and effect of start-of-injection timing and pressure history

code to solve for the chemistry during the multidimensional engine simulations. In this case, each computational cell is assumed to be a well-stirred reactor, as verified in previous studies, such as Ref. [20].

Spray models of the present study applied updated spray models, including the gas-jet model [21,22], the radius-of-influence (ROI) collision/coalescence model [23], and the mean-collision-time model [23] in order to reduce the grid-size dependency effect. Previous studies have shown that the updated spray models produce more reliable results that are relatively insensitive to grid-size in both engine simulations [21] and spray calculations in a constant volume bomb [23]. The grid-independent spray models were implemented into the KIVA-3V RELEASE 2 code, which includes the Kelvin-Helmholtz/Rayleigh-Taylor (KH-RT) spray atomization and breakup model [24] and the renormalized group (RNG) $\kappa$-$\varepsilon$ model [25] for the calculation of ambient gas flow turbulence. Details of the submodels used for the present study are listed in Table 3.

The temperature and pressure at intake valve closure were set to 450 K and 84 kPa based on WAVE calculations [26]. The other calculation conditions were the same as the experiments.

## 4 Results and Discussion

**4.1 Combustion Characteristics of a Throttled Stoichiometric Diesel Combustion.** The combustion characteristics of a throttled stoichiometric diesel operation are significantly different from those of the conventional diesel combustion because of the lower ambient gas density and no excess oxygen. In the present study the combustion characteristics of throttled stoichiometric diesel combustion were analyzed using both experiments and modeling. Figure 3 shows comparisons of calculated pressure history and the experiments at various injection timings. It can be seen that the present models predict ignition timings and peak combustion pressures quite well. Both KIVA and the experimental results show rapid combustion occurs at the early stages of combustion, which is different from previous studies which adopted high EGR [12–14] to achieve stoichiometric combustions.

In Fig. 4, which shows calculated heat release results, the portion of premixed combustion is around 65%. Reitz and co-workers [12–14] showed that the portion of premixed combustion is decreased as the equivalence ratio approaches stoichiometric because mixing is not sufficient, due to the lack of available oxygen. They reported that the portion of premixed combustion is around 50% at stoichiometric operation when around 40% EGR is used. There are several reasons for the more HCCI-like combustion of the present throttled stoichiometric diesel combustion compared with the high EGR case.

Based on the large portion of premixed combustion, it is believed that the mixture is more homogeneous compared with high EGR stoichiometric diesel combustion. In order to analyze the mixture quality, an indicator suggested by Sun and Reitz [27], was used. The inhomogeneity (normalized standard deviation or *NSD*) is defined as the normalized standard deviation of the local equivalence ratio, considering the local mass distribution as a weighting factor. The inhomogeneity is given by [27]

$$NSD = \frac{1}{\bar{\Phi}}\sqrt{\frac{\sum_{i}^{\text{No. of cells}} (\Phi_i - \bar{\Phi})^2 \delta m_i}{\sum_{i}^{\text{No. of cells}} \delta m_i}} \tag{1}$$

where

$$\bar{\Phi} = \frac{1}{\bar{\Phi}}\sqrt{\frac{\sum_{i}^{\text{No. of cells}} \Phi_i \delta m_i}{\sum_{i}^{\text{No. of cells}} \delta m_i}} \tag{2}$$

and $\Phi$ is the local atom concentration-based equivalence ratio $(2[C]+[H]/2)/[O])$.

Figure 5 shows that the inhomogeneity is around 0.8 for most injection times, which shows significantly improved mixing compared with the high EGR stoichiometric case that showed 1.3 inhomogeneity [14]. The longer ignition delay also indicates that there is enough time for mixing, as shown in Fig. 3.

The other reason for the improved mixing with throttled stoichiometric diesel combustion is the longer spray penetration. It is

Table 3 Submodels employed for the multidimensional simulations

| | |
|---|---|
| Ignition/combustion model | CHEMKIN chemistry solver |
| CHEMKIN mechanism | ERC-PRF n-heptane mechanism |
| $NO_x$ mechanism | Reduced gas research institute (GRI) mechanism |
| Soot model | Two-step phenomenological model |
| Atomization/breakup model | KH-RT model |
| Liquid/gas phase momentum coupling | Gas-jet model |
| Collision model | Radius-of-influence collision model |
| Time-step calculation | Mean collision time-step model |

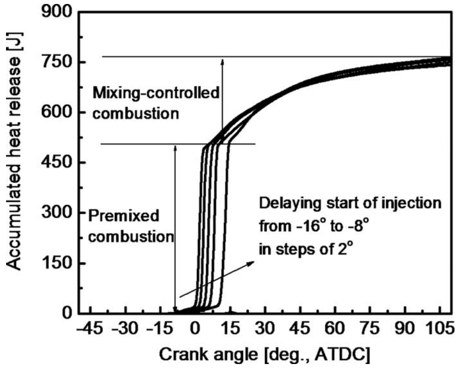


**Fig. 4 Calculated results of accumulated heat release rates. A portion of premixed combustion is around 65% for all start-of-injection timings.**

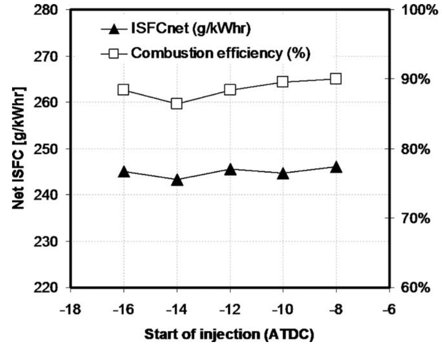


**Fig. 7 Experimental results of fuel consumption and combustion efficiency**

well-known that low ambient gas density results in a longer spray tip penetration [28]. A longer spray penetration makes a more homogeneous mixture, as shown in the local equivalence ratio contours of Fig. 6. In Fig. 6, the equivalence ratio in most of the computational cells is below 3.0. This is low compared with previous results [14] in which the peak rich equivalence ratio area was above 5.0. A longer spray penetration also contributes to the delayed start of combustion, as shown in ignition delay results of Fig. 5. With long penetration, the mixture is located over a wider region near the piston wall. This prevents the formation of a rich-mixture area and the ignition delay is increased.

Figure 7 shows the experimentally measured net indicated specific fuel consumption (ISFC) and combustion efficiency. As can be seen in this figure, the start-of-injection timing has a minimal effect on the ISFC. From Figs. 3 and 4, it can be seen that most of the heat starts to be released ATDC, even for the earliest injection case (i.e., SOI: −8 deg) because the ignition delay is quite long as described above. In addition, the combustion efficiencies, which represent the fuel energy loss during combustion due to unburned products like unburned hydrocarbon and carbon monoxide, are similar for most cases.

The overall values of the ISFC are comparable to those seen with high EGR stoichiometric diesel combustion [12,13], which were around 240 g/kW h even for optimized cases. In addition, the present throttled stoichiometric diesel engine concept has advantages in fuel consumption over advanced gasoline engines (e.g., gasoline direction injection (GDI) engines [29], particularly since the emissions (i.e., CO, $NO_x$, and HC) are manageable through the use of a three-way catalyst as efficiently as for stoichiometric gasoline engines.

Summarizing the results from Figs. 3–7, the throttled stoichiometric diesel combustion concept provides a more homogeneous mixture owing to the longer ignition delay and higher spray penetration. This retards the start of combustion to occur ATDC, which contributes to the improvement of fuel consumption over high EGR operation.

Although the present throttled stoichiometric diesel combustion concept allows the application of a well established aftertreatment technology, engine-out emissions still need to be controlled to levels manageable in aftertreatment systems.

Figure 8 shows the experimental and calculated results of engine-out emissions. For CO and $NO_x$ emissions, the KIVA prediction shows good agreement with experiments. HC and soot emissions are predicted reasonably trendwise by KIVA, although there are some quantitative discrepancies.

In Fig. 8(*a*), CO emission is decreased by retarding the injection timing. Based on the calculated results of the in-cylinder CO histories, it can be seen that CO is oxidized to $CO_2$ more quickly with retarded injection timings (see also Fig. 9). From the equivalence ratio distributions of Fig. 10, it can be seen that the spray targets the vertical area of the piston bowl edge for the early injection case (SOI=−16 deg). This leads to a locally rich region in the bowl. On the other hand, for the late injection case (SOI =−8 deg), the spray is targeted at the rounded bottom corner of the piston bowl, which leads to a more ideal distribution of the fuel. As a result, more CO is generated in the bowl for the early injection case.

From the point of view of CO it is more beneficial to retard the start-of-injection to be as late as possible to achieve low CO, while keeping similar ISFC and $NO_x$ emissions (see Fig. 8). In the present study, the injection retard limit was −8 deg due to misfire. However, it is believed that increasing the intake temperature could contribute to further reduction in CO.

In Fig. 8(*b*), the HC emissions show a similar trend to the CO emissions because the formation conditions are similar to each other [1]. Figures 8(*c*) and 8(*d*) show that the start-of-injection timing has little effect on $NO_x$ and soot emissions for the present study.

Further experimental tests were performed with the three-way catalyst employed and the −8 deg ATDC injection timing

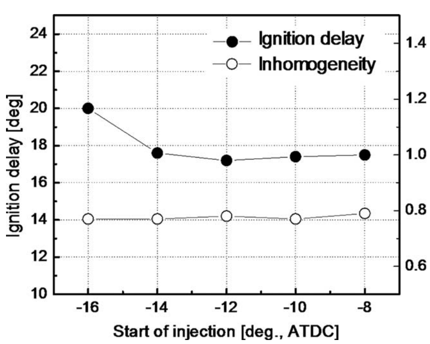


**Fig. 5 Inhomogeneity and ignition delay from KIVA results**

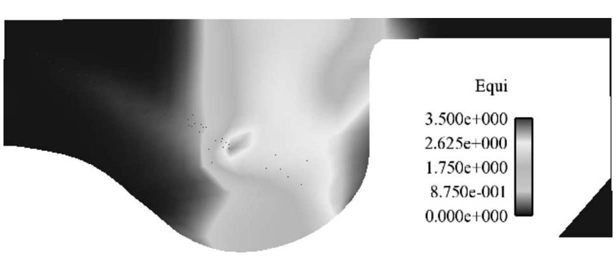


**Fig. 6 Calculated local equivalence ratio distributions at the end of injection (SOI: −8 deg)**

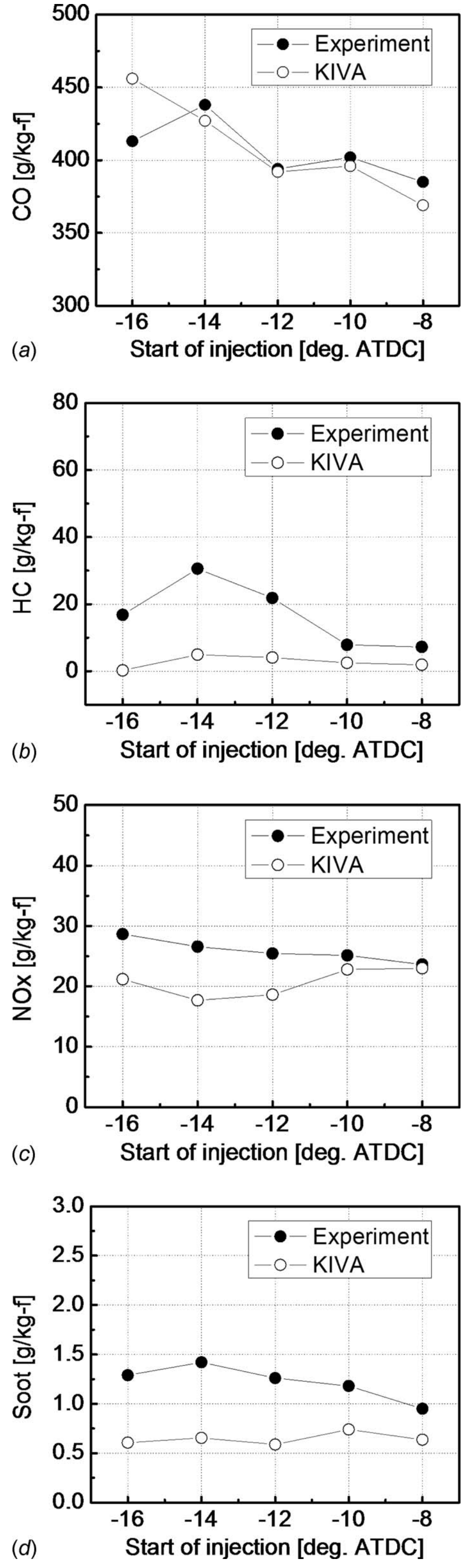


**Fig. 8 Engine-out emissions of throttled stoichiometric diesel combustion**

throttled stoichiometric case. The exhaust surge tank back pressure was set as 100 kPa and the exhaust was routed to the catalyst.

**4.2 Emission Reduction Using a Three-Way Catalyst.** In operation of the three-way catalyst, heat losses through the exhaust line cooled the exhaust gas to 175°C, which was insufficient for TWC operation. Accordingly, a heater was employed prior to the catalyst. For the results in Fig. 11 the electric heater reheated the exhaust gas up to 325°C, which is known to be an appropriate temperature for a typical automotive TWC.

The corresponding emissions results are shown in Table 4. The $NO_x$ conversion efficiency of 98.7% was achieved, which is below the U.S. 2010 standards for $NO_x$ emissions. The relatively low HC conversion efficiency might be associated with the fact

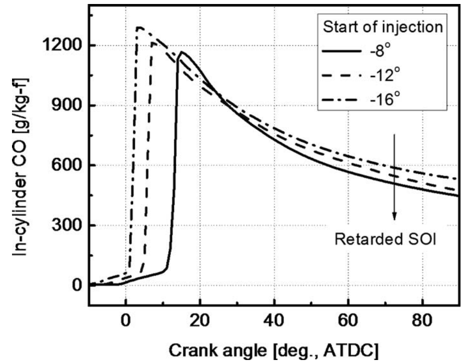


**Fig. 9 Effect of start-of-injection timing on in-cylinder pressure histories (KIVA results)**

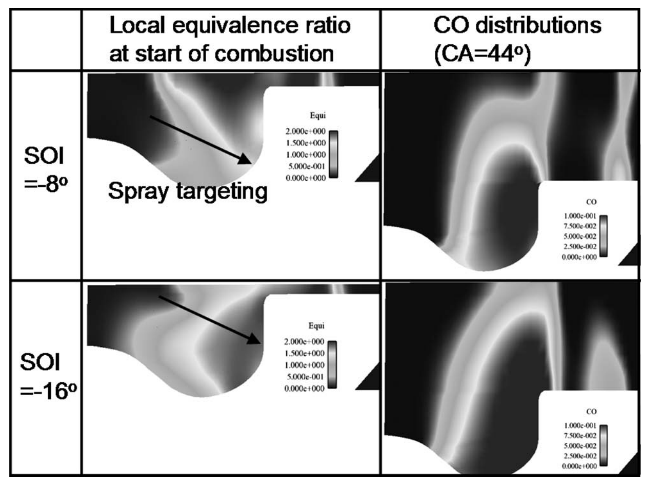


**Fig. 10 Local equivalence ratio at the start of combustion and CO distributions for −8 deg and −16 deg SOI cases**

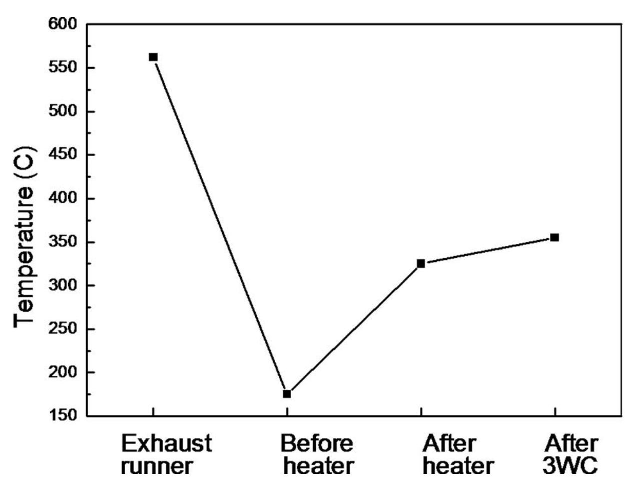


**Fig. 11 Temperatures of exhaust gas at exhaust port, inlet and outlet of a heater, and outlet of a TWC**

**Table 4 Conversion efficiencies of the three emission species and residual $O_2$ based on measurements on the inlet and outlet of a TWC**

| Species | Conversion efficiency (%) |
|---|---|
| HC | 63.2 |
| $NO_x$ | 98.7 |
| CO | 87.0 |
| $O_2$ | 90.2 |

that a substantial amount of the hydrocarbon in diesel exhaust is high-carbon number hydrocarbons ($C_4H_x$ or higher) [30]. The high residual $O_2$ ($\sim 10{,}000$ ppm) did not seem to affect the TWC performance. Also, for controlling soot emissions a DPF could be integrated in the exhaust system.

## 5 Conclusions

The combustion and emission characteristics of throttled stoichiometric diesel combustion were studied experimentally and numerically in the present study. By throttling the intake pressure in a diesel engine, the combustion and emission characteristics are changed significantly compared with boosted intake pressure high EGR cases. In addition, a three-way catalyst was adopted for the simultaneous reduction in $NO_x$, CO, and HC. The following conclusions can be drawn based on the experimental and modeling results.

1. By throttling the intake pressure, a more homogeneous mixture is provided mainly due to the long ignition delay and increased spray penetration. This contributes to an increase in the portion of premixed heat release in the combustion process.
2. The fuel consumption of throttled stoichiometric diesel combustion is comparable to that obtained with high EGR stoichiometric diesel combustion, and it has some advantage over advanced gasoline engines like GDI engines.
3. CO emission is decreased by retarding injection timing because the spray optimally targets the bowl, which guides the in-cylinder fuel distribution.
4. The use of a three-way catalyst provided 98.7% $NO_x$ conversion efficiency, which successfully lowered $NO_x$ below U.S. 2010 $NO_x$ levels.
5. Although it did not affect the TWC performance, a relatively high residual $O_2$ level of 1% was formed in the exhaust from the present stoichiometric diesel operation. This could require a modification to the current residual-$O_2$ based air-fuel ratio estimates obtained with a lambda sensor.


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## Nomenclature

$m_i$ = total mass in calculation cell $i$

$P_{inj}$ = injection pressure

$\varphi$ = equivalence ratio

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