

# A Computational Study of the Effects of EGR and Intake-Pressure Boost on DME Autoignition Characteristics over Wide Ranges of Engine Speed

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## ABSTRACT

This study has been computationally investigated how the DME autoignition reactivity is affected by EGR and intake-pressure boost over various engine speed. CHEMKIN-PRO was used as a solver and chemical-kinetics mechanism for DME was utilized from Curran's model. We examined first the influence of EGR addition on autoignition reactivity using contribution matrix. Investigations concentrate on the HCCI combustion of DME at wide ranges of engine speeds and intake-pressure boost with EGR rates and their effects on variations of autoignition timings, combustion durations in two-stage combustion process in-detail including reaction rates of dominant reactions involved in autoignition process. The results show that EGR addition increases the combustion duration by lowering reaction rates. It was also found that autoignition timings were very sensitive to boost pressure due to boost pressure enhances the reactivity of intermediate species but combustion durations dominantly depend on the EGR addition. Also, high engine speed under EGR addition increases the burn duration greatly. Finally, the combined effects of EGR and boost pressure over wide ranges of engine speed are showed that it is the beneficial method to operate HCCI engine without knock at high load due to substantial reduction of peak of heat-release rate by controlling low temperature heat release.

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## INTRODUCTION

Homogeneous charge compression ignition (HCCI) engine is named as the candidate of next generation internal combustion engine with the high efficiency of the CI engine and the very low emissions of the SI engine [1, 2, 3, 4, 5, 6, 7]. Known benefits of HCCI are near-zero nitrogen oxides (NOx) and PM emissions. However, several technical matters have to be solved before its widespread production. Among these, controlling the rate of energy release and ringing [8] at high loads have been main problems. The use of cooled EGR (external EGR) was found to slow down combustion by the means of controlling the heat release over wide ranges of engine speed, lower the peak pressure, and more expand the high load limit of operation [9]. A combination of increase of specific heat capacity and reduction of O<sub>2</sub> concentration associated with EGR addition results in suppression of autoignition and combustion-phasing retard, allowing high-load operation without knock [10, 11, 12, 13, 14]. However, too much amount of EGR results in lower power output and increase the unburned hydrocarbon (HC) and carbon monoxide (CO) emissions since the constituents

forming EGR suffer the rapid burning rate. Therefore, one way to increase the load range is to increase the intake-pressure boost which enhances the autoignition reactivity of the fuel. Controlling the combustion phasing is particularly important under boosted conditions since the greater charge mass with boost increases the amount of pressure rise [15, 16, 17, 18, 19]. Due to the appropriate strategies of EGR and intake-pressure boost have the capability of extending the HCCI operation range to higher loads and further potential to be used in commercial engines. The principal and control mechanism of EGR on HCCI autoignition have to be elucidated in-detail for chemical kinetics across relatively wide ranges of operating parameters.

The main objective of this study is to computationally investigate the effects of EGR and boost pressure over the wide ranges of engine speed on DME HCCI autoignition. The "Contribution matrix to heat release" and "Absolute heat-release rate" of important elementary reactions are plotted for each fuel to identify the underlying mechanism by comparing various cases, which are: 1) Cases between no EGR addition

and EGR addition over wide ranges of engine speed, and 2) Cases between EGR addition with no boost pressure and EGR addition with boost pressure over wide ranges of engine speed.

## COMPUTATIONAL APPROACH

### 1. Chemical-Kinetics Modeling Setup

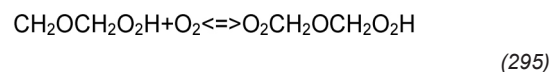
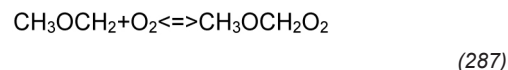
The computational investigations have been conducted using the single-zone model of CHEMKIN [20,21] included in CHEMKIN-PRO [22]. The single-zone model treats the in-cylinder charge as a single lumped mass with uniform composition and thermodynamic properties. Heat-transfer and blow-by effects were not included. Compression / expansion was modeled according to the standard slider-crank relationship [23], using the geometry and specifications of the single-cylinder HCCI engine shown in Table 1. The calculation starts from the intake valve close (IVC) of 136° bTDC to the exhaust valve open (EVO) of 125.4° aTDC. The single-zone model allows relatively short computational times even with the detailed chemical-kinetic mechanisms, so numerous changes in operation conditions can be readily examined. The fuel used was di-methyl ether (DME) whose chemical kinetics mechanisms and thermodynamic parameters were used from Lawrence Livermore National Laboratory (LLNL) [24,25] and its properties showed in Table 2. DME fuel is considered a promising clean alternative fuel for ground transportation vehicles, and it can be a substitute for conventional diesel fuel in a compression ignition diesel engine [26]. The molecular ratio of air was as follows N<sub>2</sub>:O<sub>2</sub>:Ar=78:21:1, and the EGR gas was composed from CO<sub>2</sub> and H<sub>2</sub>O. For this modeling work, no attempt is made to capture the effect of trace hydrocarbon species such as carbon monoxide (CO), hydrocarbons (HC) and partially-oxidized hydrocarbons encountered experimentally in real EGR.

The heat release of an oxidation process of DME which has cool flame is composed of four ranges, cool-flame, negative temperature coefficient (NTC), thermal ignition preparation (TIP) and thermal-ignition (TI) range [27]. Among these ranges, the first two belong to low temperature heat release (LTHR), and the last two belong to high temperature heat release (HTHR). Based on above ranges, a significant amount of heat is released without discussion above, the key timings of DME oxidation as illustrated in Figure 1 are as follows. The first time heat release rate (HRR) reaches 1% of total heat release is viewed as the start timing of the cool flame. As the reproduction of OH radicals will be terminated as the NTC stage is reached, the first peak timing of OH mole fraction can be viewed as the end of the cool flame, thus, the start of NTC. The turning point of OH radical mole fraction after the first peak is considered as the end of the NTC stage. When the NTC stage ends, the oxidation process will enter the thermal ignition preparation stage, during which the OH radicals will accumulate again. Finally, the cross timing of the mole fraction of H<sub>2</sub>O<sub>2</sub> and OH is viewed as the start of thermal ignition

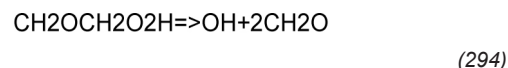
because the decomposition of H<sub>2</sub>O<sub>2</sub> into OH radicals is the initiator of the thermal explosion. The timing when HRR returns to 99% of total heat release is considered as the end of HTHR.

### Reaction Mechanisms of DME

Reactions involved dominantly in autoignition of DME were divided in three main groups which are fuel series reactions, H<sub>2</sub>O<sub>2</sub> loop reactions and hydrogen-oxygen (H<sub>2</sub>O<sub>2</sub>) system reactions [27,28]. Fuel series reactions are dominant in cool-flame range, which is initiated by the primary O<sub>2</sub> addition Reaction(287) and then secondary O<sub>2</sub> addition Reaction(295).



The transition from the cool-flame range to the NTC range is controlled by the competition of the secondary O<sub>2</sub> addition Reaction(295) to generate 2OH in consequence, and the decomposition Reaction(294) to generate OH.



H<sub>2</sub>O<sub>2</sub> loop reactions play important role in the initiation of thermal ignition by supplying heat rather than radicals.

Table 1. Engine specification.

|                    |             |
|--------------------|-------------|
| Displaced volume   | 498 cc      |
| Stroke             | 92 mm       |
| Bore               | 83 mm       |
| Connecting Rod     | 145.8 mm    |
| Compression ratio  | 14.5:1      |
| Number of Valves   | 2           |
| Inlet Valve Close  | 136° bTDC   |
| Exhaust Valve Open | 125.4° aTDC |

Table 2. Fuel properties.

| Property                    | DME                                | Diesel  |
|-----------------------------|------------------------------------|---------|
| Chemical structure          | CH <sub>3</sub> -O-CH <sub>3</sub> | -       |
| Critical temperature [K]    | 400                                | 708     |
| Critical pressure [MPa]     | 5.37                               | 3.00    |
| Cetane number [-]           | >55                                | 40-50   |
| Boiling point at 1 atm [K]  | 248.1                              | 450-643 |
| Lower heating value [MJ/kg] | 27.6                               | 42.5    |

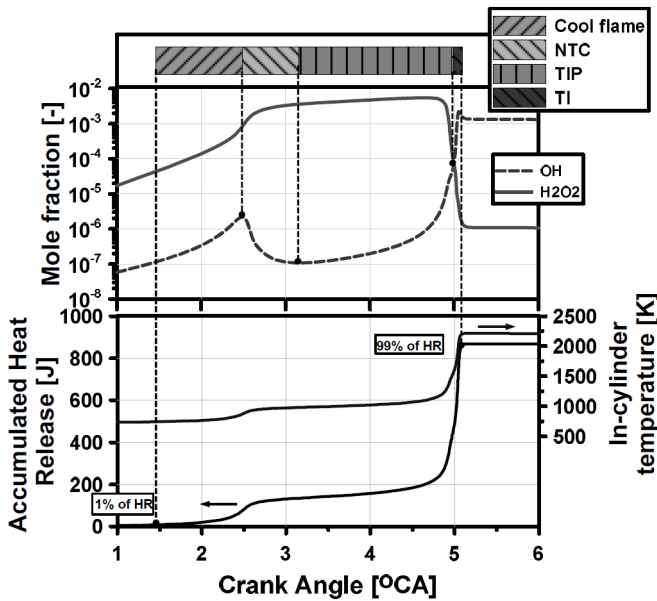
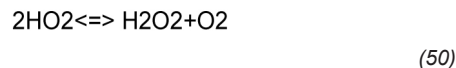
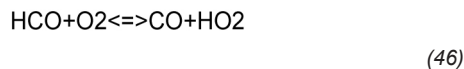
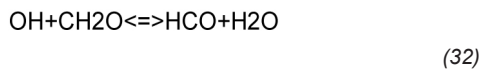
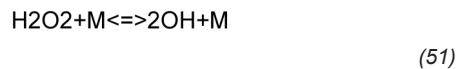


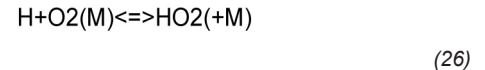
Figure 1. Definition of key combustion timings.

Reaction loop begins at 950K, which is the transition from the NTC range to the thermal-ignition preparation range. Enhanced H2O2 loop shortens ignition delay. Therefore, the transition process from NTC to thermal ignition preparation depends on strongly from loop reaction.



Among the loop reactions, [Reaction\(51\)](#) has special behavior whose reaction rate solely increases during the increase of temperature at beginning of NTC range while others ([Reaction 32](#), [46](#), and [50](#)) begin to decrease. Abstraction with HO2 causes the production of hydrogen peroxide (H2O2) which gradually increases in concentration until the mixture reaches a temperature of approximately 1000K. Above 1000K, the oxygen-oxygen bond in H2O2 breaks more readily causing the [reaction 51](#), which rapidly releases a large amount of OH radicals. As a result of this reaction which proceeds more quickly above 1000K, the previously stable hydrogen peroxide molecules act as a sudden source of OH radicals which consume the fuel molecules more quickly, leading to rapid heat release. The role of thermal ignition preparation reactions is to increase the temperature to initiate the thermal ignition. The breakdown of hydrogen peroxide into OH radicals and their

subsequent reactions causes increasing temperature which further accelerates the breakdown of hydrogen peroxide [19]. This leads to an autoignition event that increases the temperature to above 1500K (in this study) where thermal ignition take place through branching chain reactions in the hydrogen oxygen reaction mechanism. Thermal ignition initiation is the competition between [Reaction 8](#) and [26](#). The [Reaction\(8\)](#) prevails [Reaction \(26\)](#) above 1500K.



### Contribution Matrix to Heat Release

Autoignition process can be simplified by the extracting important reactions from detailed chemical kinetics mechanisms using “contribution matrix to heat release” [27,28] as shown in [Eq.1](#).

$$\text{CHR}_{j,T} = \frac{\text{HR}_{j,T}}{\sum_{j=1}^N \text{abs}(\text{HR}_{j,T})} \cdot 100\% \quad (1)$$

Here,  $\text{CHR}_{j,T}$  is the contribution ratio of  $j^{\text{th}}$  elementary reaction to heat release at a transient temperature  $T_t$ .  $\text{HR}_{j,T}$  is the heat release rate by the  $j^{\text{th}}$  elementary reaction at  $T_t$ . This study utilized the data for the value of contribution ratio to heat release of important elementary reactions above 3% at  $T_t$ .

### 2. Definition of EGR Rate

The EGR gas composition was the same with that of complete combustion products as CO2 and H2O. These are named as complete stoichiometric products (CSP). EGR was defined by the mixture of CSP and remained gases from previous cycle which was defined in the paper by Jung et al. [18]. This mixture will impact greatly since combustion behavior of HCCI does depend on directly from mixture conditions. In this study, there will be no data for CO and HC since these are difficult to obtain the precise amount during the engine operation. Therefore, EGR rate was calculated by the [Eq. 2](#) as follow:

$$\text{EGRrate} = \frac{n_{\text{EGR}}}{n_{\text{EGR}} + n_{\text{air}}} \cdot 100\% \quad (2)$$

$n_{\text{EGR}}$  and  $n_{\text{air}}$  are the mole fractions of EGR and air, respectively.

### 3. Knock and Misfire Limits

For this study, the ringing correlation developed by Eng [8] is used to quantify the knock level:

$$\text{Ringing Intensity} \approx \frac{1}{2\gamma} \cdot \frac{\left(0.05 \cdot \frac{dP}{dt, \max}\right)^2}{P_{\max}} \cdot \sqrt{\gamma R T_{\max}} \quad (3)$$

Eq.(3) shows that the ringing intensity is proportional to the square of the absolute maximum pressure-rise rate (PRR) (in kPa/ms). ( $P_{\max}$  should be given as kPa, whereby Eq.(3) gives the ringing intensity in kW/m<sup>2</sup>. The speed of sound comes in through the square root expression, and should be in m/s.) The use of a time based pressure-rise for computing ringing/knock is justified by the fact that the acoustic time scales are independent of engine speed. 5MW/m<sup>2</sup> was chosen as the limit for allowable ringing.

The beginning of the main heat release marks the onset of hot chemistry with breaks down of H<sub>2</sub>O<sub>2</sub> at temperature around 1100K. Refer to the maximum temperature, the onset of misfire reactions can be judged when reaching the temperature below 1100K [30].

## RESULTS

In order to investigate systematically the fundamental effects of EGR, intake-pressure boost and engine speed, and their correlation on HCCI combustion and its autoignition, influence of EGR was confirmed at 1200rpm and naturally aspirated (NA) operation. Continuously, EGR influence was confirmed on the operation of boosting as 0.1MPa and 0.2MPa in increment of 0.025MPa on 1200 rpm and 2100rpm. In final, engine speed was changed from 600 rpm to 2100rpm by the increase of 300rpm over EGR to clarify the mechanism of autoignition. Throughout this study, CA50 was focused to set at the 5°C aTDC since later combustion phasing from high amount of EGR results the lower power output as well as higher hydrocarbon (HC) and carbon monoxide (CO) emissions due to cooling effect of expansion.

### 1. Effects of EGR Addition with Naturally Aspirated Operation

As outlined above, this section investigates the effect of EGR addition on autoignition mechanism of HCCI combustion fueled with DME. Figure 2 shows the required intake temperatures, combustion duration and key combustion temperatures as a function of EGR rates. As can be seen in top of figure, intake temperatures were increased along with the increase of EGR rate to achieve the CA50 at 5°C aTDC, which was a reason to compensate the reduction of oxygen concentration. As can be seen from combustion duration, autoignition was occurred in advance at higher EGR rate cases, in which cool flame was

shortened but NTC was lengthened. It was clear to see that TIP was lengthened noticeable to other regimes of autoignition. Although TI was occurred identical time at 50% EGR case, its duration was much longer than other lower EGR rate cases. Generally, combustion duration was increased and autoignition reactivity was slowed down as the increase of EGR. In case of key combustion temperatures, the only increased temperature was start temperatures of cool flame which were increased slightly as 22K due to higher intake temperature at EGR<sub>rate</sub>=50% compared to no EGR case but other key temperatures were decreased clearly which might be caused from the reason of the slowed autoignition reactivity. Start temperatures of thermal ignition (TI) were decreased by 48K. As mentioned above, shortened durations of cool flame could be related to the increase of EGR rate. It was clear to see that occurrence times of LTHR were advanced before TDC. However, NTC ranges were lengthened since their occurrence temperatures were getting decreased. There is one phenomena very interesting to investigate further meaning which is clearly lengthen of TIP. It might be the reason of the decreased start temperature of TI. As mentioned in many studies, EGR suppresses the heat formation rate before thermal ignition [9-10]. Therefore, TI length was getting increased as the increase of EGR rate. Figure 3 shows the effects of EGR addition on PRR reduction. It was typically explained by the reduced combustion temperature from less amount of oxygen concentration. To understand in depth the effects of EGR addition, no EGR and 50% EGR condition was chosen to compare and its combustion characteristics are shown in Figure 4. EGR reduces the in-cylinder pressure and temperature which results the low HRR. Although the effects of EGR was briefly explained above, its mechanism on autoignition was still unclear. It is important to understand the increase of combustion duration by reduced combustion temperature. In order to clarify the underlying mechanism, the heat release of elementary reactions involved in autoignition were separately considered with autoignition regimes. Therefore, contribution matrix to heat release in which reactions were above the threshold as 3% was utilized and it gives the possibility to distinguish the important reactions participated in autoignition process of DME HCCI combustion. As can be seen in the Figure 5, absolute heat release for overall dominant reactions and rates of those reactions in separate autoignition regimes for no EGR and EGR=50% were selected for comparison. As can be seen from the legend at the top left side of figure, absolute HRR is black line, which was higher abs.HRR and longer temperature duration at no EGR case compared to 50% EGR case. To better understand this phenomena, elementary reactions were divided into three main groups as fuel-series, H<sub>2</sub>O<sub>2</sub> loop, and H<sub>2</sub>O<sub>2</sub> system reactions [27,28].

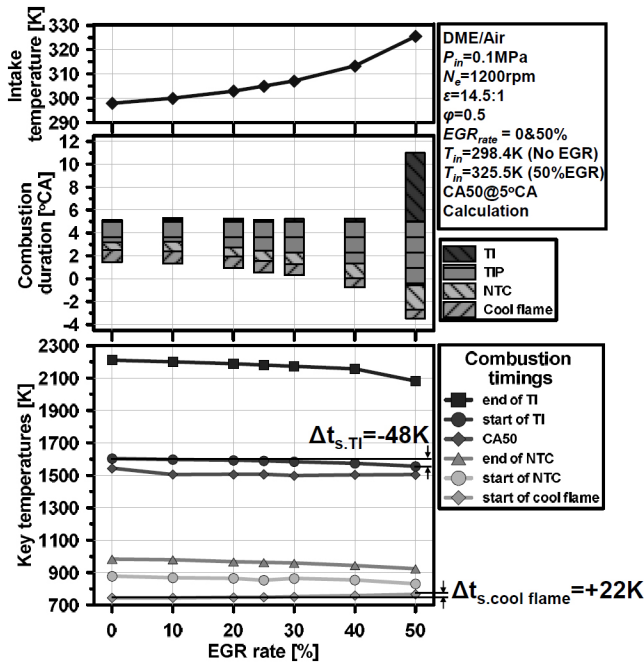


Fig. 2. Effect of EGR rate on required intake temperature, combustion duration and key combustion temperatures at 1200rpm.

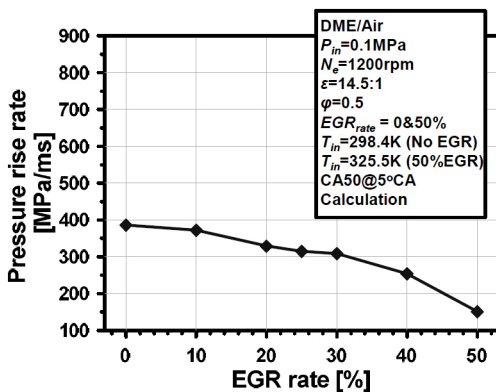


Fig. 3. Effect of EGR on pressure rise rate at 1200rpm.

### Cool-Flame and NTC Range

The amount of LTHR in higher EGR addition was less than no EGR addition which might be the low amount of oxygen. Although, cool flame was occurred before TDC at 50% EGR, its occurrence temperature was lower than that of no EGR case. Therefore, both rates of reverse and forward reactions were lower. Among the fuel-series reactions, primary O<sub>2</sub> addition by 287 reaction and secondary O<sub>2</sub> addition by 295 reaction are dominant in cool flame. Reaction 294 is transition reaction from cool-flame to NTC which suppresses the reaction rate. The equilibrium of these reactions shift toward the reactants side and the addition of O<sub>2</sub> to the alkyl radical is almost completely extinguished with the higher temperatures [31]. Black lines are for no EGR while grey lines are of 50% EGR at NA operation. The temperature range for cool flame

surrounded between 745K and 880K for no EGR operation while it was started at 767K and terminated at 830K to NTC range for 50% EGR. It was thought that EGR shortens the temperature range of cool flame. In case of NTC, it was terminated at 983K and 924K for no EGR and EGR case, respectively. The lower transition temperature of cool flame to NTC was a reason for longer duration of NTC in Fig.2. In order to comprehend the underlying mechanism of this event, reaction rates of both reverse and forward were plotted along with the in-cylinder temperature for autoignition ranges. Reactions went as similar trend to absolute HRR within these regions. Absolute HRR of primary O<sub>2</sub> addition reaction (287) was higher at no EGR than that of EGR case. Around 860K for no EGR, decomposition reaction (294) was crossed with secondary O<sub>2</sub> addition reaction (295) and went upward since its forward reaction rate was increased, which was taken place around 815K for EGR case. Therefore, reaction (294) was responsible for the occurrence of NTC, which was solely increased at the transition region of NTC from cool flame. In both cases, reverse reaction of 294 was not taken place. During the NTC range, rates of all reactions were decreased and terminated at 980K and 920K for no EGR and EGR case, respectively. Mainly this trend was comparable with combustion duration. In both cases, the minimum transient temperature of reaction 294 for HRR after the first peak was matched up to the end of NTC.

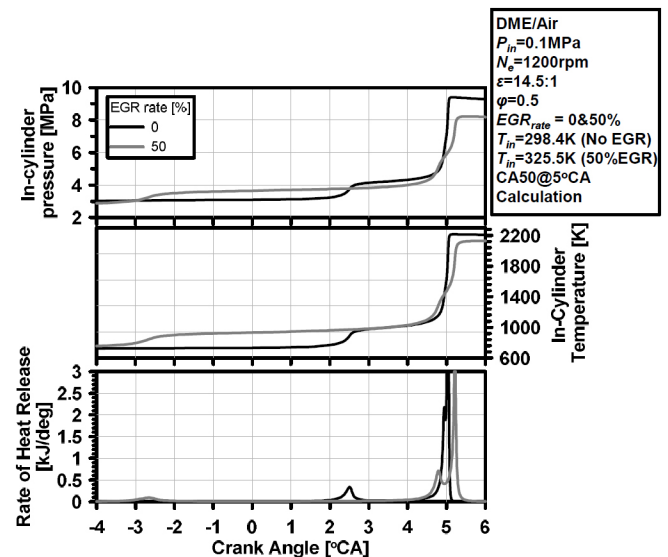


Fig. 4. Profiles of in-cylinder pressure, temperature and heat release rate for the case of no EGR and 50% EGR.

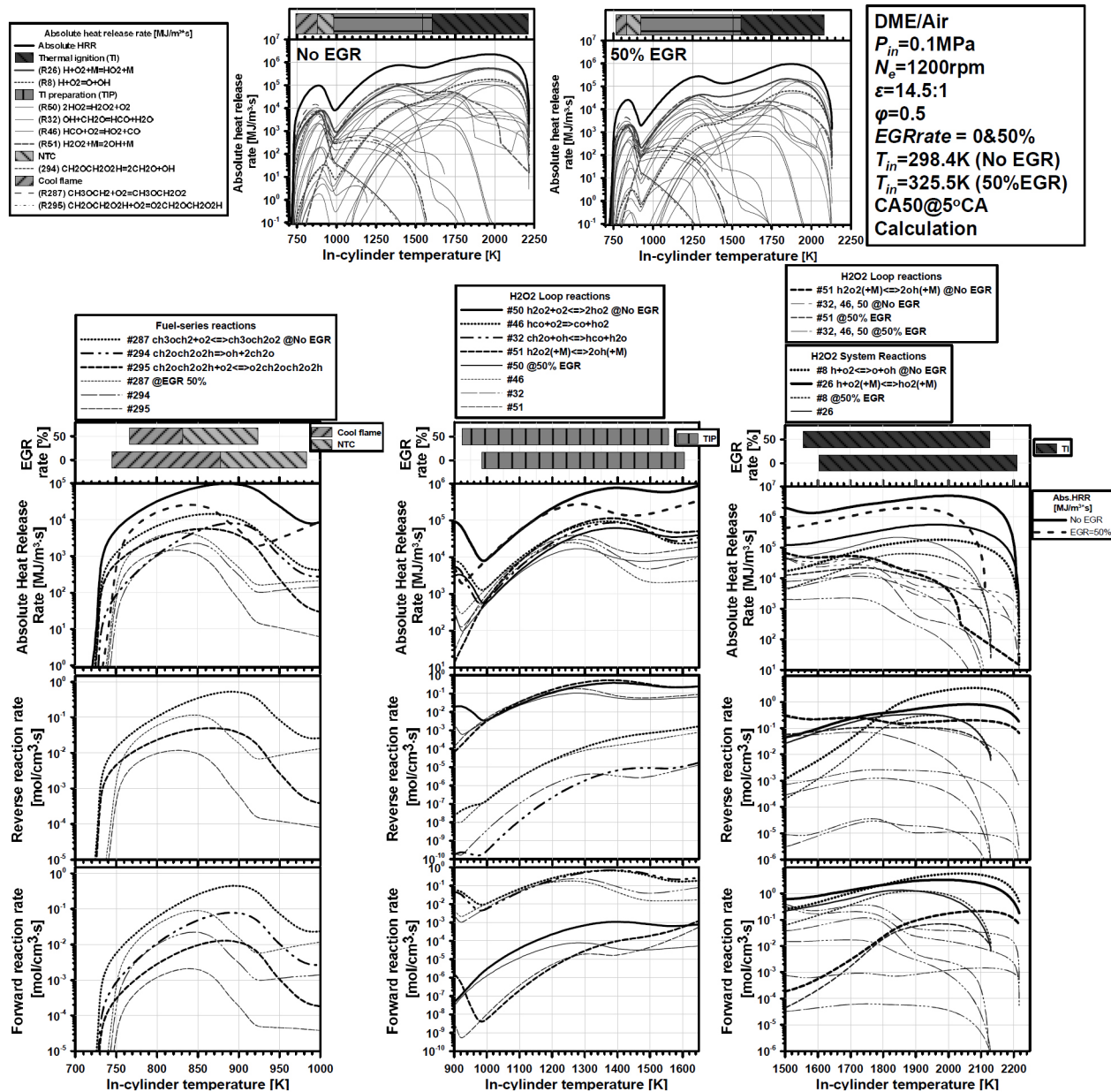


Fig. 5. Absolute HRR and reaction rates for dominant reactions in autoignition of DME HCCI combustion in case of no EGR and 50% EGR.

### Thermal-Ignition Preparation and Thermal Ignition

The role of TIP reactions is to increase the temperature to initiate the TI. After the fuel series reactions, H<sub>2</sub>O<sub>2</sub> loop reactions were the main contributor to TI range in TIP range, which plays an important role in the thermal ignition by supplying heat rather than radicals. During the NTC range, reaction rates and heat release rates of almost all reactions decreased but the only reaction that was increased without falling down along with the increase of in-cylinder temperature was H<sub>2</sub>O<sub>2</sub> decomposition reaction (51) to generate OH. TIP begins around 980K and 925K after NTC in both cases. At 50% EGR case, NTC was terminated at lower temperature and TIP was started and went through lower reaction rates, in which forward reaction rates were decreased as the increase of in-cylinder temperature. This is the reason for slowed down of autoignition with lower heat release and longer burn duration at

TIP range. It can be also confirmed in combustion duration in Fig. 2, where TIP was lengthened evidently at EGR case. In TI range, although there are a number of reactions contributed as plotted in the absolute heat release graph on top of figure, hydrogen-oxygen system reaction was initiated by the decomposition of H<sub>2</sub>O<sub>2</sub> and the increase of OH, in which the competition of branching chain reaction (8) and HO<sub>2</sub> recombination reaction (26) are dominant along with temperature. As the temperature increases after TIP, reaction (51) of H<sub>2</sub>O<sub>2</sub> loop was also contributor to take place of thermal ignition among the other reactions, of which reaction rates are higher than other reactions of loop. Reverse reaction rates of EGR had higher than that of no EGR case while it was inverse at forward reaction rate. This higher reverse reaction rate of H<sub>2</sub>O<sub>2</sub> loop reactions at EGR case might be responsible for evidently longer TIP duration. At high EGR rate case,