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A numerical study on the quasi-steady spray and soot characteristics for soybean methyl ester and its blends with ethanol using CFD-reduced chemical kinetics approach

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Abstract

This work numerically examines the quasi-steady spray combustion and soot development for soybean methyl ester (SME) and SME-ethanol blends (S90E10, S70E30). A validated reduced ethanol mechanism (37 species and 149 reactions) was formulated using a temperature sensitivity analysis under auto-ignition and jet-stirred reactor conditions. At initial pressures between 10.0 bar and 60.0 bar, initial temperatures between 750 K and 1350 K and equivalence ratios between 0.5 and 2.0, the ignition delays and key species profiles (C₂H₅OH, CO₂, O₂) of the reduced mechanism deviated by 0.5 order and 40%, respectively as compared to the experimental measurements. Subsequently, the reduced ethanol mechanism was combined with a reduced biodiesel mechanism to form a surrogate mechanism (102 species and 446 reactions) for biodiesel-ethanol blends and integrated into OpenFOAM for spray combustion modelling. Under reacting spray conditions at a constant ambient density of 22.8 kg/m³ and ambient temperatures of 900 K and 1000 K, the spray penetrations for SME-ethanol blends were shortened by 35.5% (maximum difference). Smaller flame areas with 60 K higher local...
flame temperature were obtained. Due to a 20% decrease in acetylene mass fractions and soot formation rates, the peak soot volume fractions for SME-ethanol blends were 19.6% lower.

*Keywords:* ethanol, reduced chemical kinetics, SME, soot, spray combustion
Introduction

Despite various approaches such as different injection strategies [1–5] and varying initial exhaust gas recirculation compositions [4–6] to address diesel engine emissions, alternative fuels are still sought-after as a solution to this problem [7]. Furthermore, the continuous search of alternative fuels is also driven by the depletion of fossil fuel reserves at an alarming rate due to global industrialisation and increased use of automobiles [8]. Current research efforts are focussed on alcohol fuels as an additive to diesel and/or biodiesel fuels since alcohol fuels reduce the emission levels of soot/particulate matter and also improves engine combustion due to higher volatility and oxygen (O₂) content [9,10] of the alcohol fuels.

Among the wide range of alcohol fuels, it is found that the use of ethanol (C₂H₅OH) fuel in internal combustion engines has led to improved combustion [11,12] and reduced life-cycle greenhouse gas emissions [13] due to the additional O₂ molecules [11,12], higher volatility [14] and increased latent heating properties of the fuel [14]. Additionally, ethanol fuel also has good compatibility with the existing propulsion and energy-generation devices [15], whereby further engine modification is not required when a low blend level of ethanol with diesel or biodiesel fuel is utilised [13]. Apart from that, the production process of ethanol fuel is comparatively more sustainable than other alcohol fuels since it is produced from the alcoholic fermentation of sugar from vegetable materials [16]. Although alcohol fuels with larger carbon numbers such as butanol (C₄H₉OH) and iso-pentanol (iC₅H₁₁OH) fuels have been gaining more attention recently, ethanol fuel is still favoured and widely used in countries like the United States, Brazil, India and China [15].

Many studies have been conducted to understand the combustion and emission behaviours of ethanol fuel when it is used in different engine setups. Generally, the addition of ethanol fuel in biodiesel combustion contributed to retardation in the ignition. Experimentally,
Lapuerta et al. [13] investigated the auto-ignition behaviours for different blends of ethanol and biodiesel, which was a mixture of methyl esters of palm (PME) and soybean (SME), in a constant volume combustion chamber operated at ambient pressures of 6.0 bar to 21.0 bar and ambient temperatures of 535 K to 602.5 K. As the percentage of ethanol increased to 75%, the ignition delay (ID) periods measured for the biodiesel-ethanol blends at the tested conditions were prolonged by approximately 33 times. Nevertheless, the emissions for the biodiesel-ethanol blends were not reported [13]. Meanwhile, at a diesel engine speed of 1800 rev/min and a load range of 0.8 bar to 7.0 bar, the ID period obtained for the biodiesel-ethanol blend was extended by 2 to 3 crank angle degrees as compared to that of the biodiesel [17]. A similar observation has also been recorded by Shudo et al. [18], where the ID periods for the PME-ethanol blends were extended according to the increase of ethanol content in a 4-stroke open chamber diesel engine. Tutak et al. [19] also found out that the ID period for a biodiesel blend with 40% ethanol was elongated by 25.7%. In terms of emissions, reduced soot/particulate matter/smoke emissions were found for the biodiesel-ethanol blends. For instance, a 2-factor reduction was obtained when comparing the smoke measured for 60% PME and 40% ethanol against that of the PME, at a brake mean effective pressure of 5.0 bar [18]. However, for a diesel engine fuelled with a biodiesel-ethanol blend of 85%-15%, at a rated power output of 8.95 kW and an engine speed of 3000 rev/min [20], the unburned hydrocarbons were approximately doubled. Apart from these, the combustion and emissions behaviours for biodiesel-ethanol fuel blends in diesel engine were also analysed numerically. For example, An et al. [21] reported an extension in the ID periods and a decrease in soot by 38% for a blend of 80% waste cooking oil biodiesel and 20% ethanol at a diesel engine speed of 2400 rev/min. Despite these works [13,17–21], to the authors’ best knowledge, the understanding of the quasi-steady spray combustion and emissions behaviours for biodiesel-ethanol fuel blends is limited.
As such, this work aims to analyse the development of quasi-steady spray combustion and soot formation/oxidation for SME and SME-ethanol blends, i.e. S90E10 and S70E30 under reacting spray conditions, using an open-source computational fluid dynamics (CFD) code, OpenFOAM version 2.0.x. First, a validated reduced chemical kinetic mechanism for ethanol which includes auto-ignition and extinction features is formulated using the temperature sensitivity analysis in CHEMKIN-Pro. The reduced mechanism for ethanol is then combined with a multi-component biodiesel surrogate mechanism (methyl decanoate, \( \text{C}_{11}\text{H}_{22}\text{O}_2 \) and methyl-9-decenoate, \( \text{C}_{11}\text{H}_{20}\text{O}_2 \)) [22] to formulate a combined surrogate mechanism for the biodiesel-ethanol blend. Subsequently, the quasi-steady spray combustion and soot processes for SME and SME-ethanol blends, namely S90E10 and S70E30 are simulated using the combined surrogate mechanism. The evolutions of the spray combustion and soot formation/oxidation such as liquid penetration, ID periods, spray/flame distributions and rates of soot surface growth are elucidated for S90E10 and S70E30, and finally compared against those of the baseline SME fuel.

2. Formulation and validation of the reduced chemical kinetic mechanism for ethanol

2.1 Reduction of chemical kinetic mechanism for ethanol

Various forms of chemical kinetics including both detailed and reduced mechanisms for ethanol have been reported in the literature. One of the earliest detailed mechanisms for ethanol was built by Marinov [23]. The detailed mechanism [23] which contained 56 species and 351 reactions was validated for auto-ignition, extinction as well as the laminar flame speed at pressures from 1.0 bar to 8.0 bar, temperatures from 300 K to 1700 K and equivalence ratio (\( \varphi \)) from 0.5 to 2.0. Apart from that, Leplat et al. [24] developed and validated a detailed mechanism for ethanol with 36 species and 252 reactions, under both the shock tube and jet-
stirred reactor (JSR) conditions, at low pressures between 0.1 bar and 4.5 bar and $\phi$ between 0.25 and 2.0. Although good levels of agreement against the experimental measurements and detailed mechanism predictions were obtained, the reduced mechanism was not further applied for multi-dimensional CFD modelling. These detailed mechanisms [23,24] are still considerably large in size due to the large number of reactions involved, which subsequently lead to an increase in the computational runtime.

Therefore, reduced mechanisms containing key species and reactions pertinent to the in-cylinder combustion and emissions phenomena have been formulated to facilitate efficient CFD simulations. Maurya and Akhil [25] developed a reduced ethanol mechanism of 47 species and 272 reactions. When compared to the experimental measurements and detailed mechanism predictions, the maximum in-cylinder pressures, heat release rates and ID periods at air-fuel ratios of 2 to 6 were replicated by the reduced mechanism, but with high deviations. Nevertheless, this reduced mechanism [25] was only examined under homogenous charge compression ignition (HCCI) conditions, which are leaner than those of the diesel engine. Similarly, the 28-species reduced mechanism for ethanol by Bhagatwala et al. [26] was only limited to HCCI conditions, despite reasonable agreement with the experimental measurements. More recently, a reduced ethanol mechanism with 31 species and 66 reactions was built by Millán-Merino et al. [15]. Under various conditions of auto-ignition, laminar flame and extinction, the reduced mechanism reasonably reproduced the ID periods and flame propagations, except for several soot precursors such as acetylene ($\text{C}_2\text{H}_2$) and ethylene ($\text{C}_2\text{H}_4$) [15].

Due to these reasons, a reduced mechanism for ethanol was formulated in this work. The detailed mechanism for ethanol proposed by Marinov [23] was selected as the base mechanism for the reduction. The Arrhenius reaction rates for selected elementary reactions in the detailed mechanism [23] were optimised in order to improve the predictions of auto-ignition
and extinction characteristics for ethanol [22,27,28]. A sensitivity analysis was performed using CHEMKIN-Pro in order to identify pertinent elementary reactions for the optimisation of the Arrhenius rate constants. Here, the absolute temperature sensitivity coefficients were calculated based on the pre-exponential factors (A-factor) in the Arrhenius reaction rate expressions for all elementary reactions. Then, the sensitivity coefficients were normalised using Equation 1. Elementary reactions pertinent to the fuel oxidation and/or dissociation with the highest normalised coefficients were considered most sensitive and selected for the optimisation of the Arrhenius rate constants [29,30]. Based on the sensitivity analysis taken at the point of ignition, C$_2$H$_5$OH + HO$_2$ = CH$_3$CHOH + H$_2$O$_2$ associated to the oxidation of ethanol was identified with the highest sensitivity among other elementary reactions. Thus, the pre-exponential factor (A-factor) in the Arrhenius reaction rate equation for this reaction was calibrated from 8.2 x 10$^3$ mol cm s K to 4.2 x 10$^4$ mol cm s K in order to replicate the experimental measurements [24]. Figure 1(a), (d) and (g) shows that a maximum under-prediction of 42.2% is obtained when comparing the C$_2$H$_4$ mole fractions at $\phi$ of 0.6, 1.0 and 2.0 predicted by the optimised detailed mechanism against those of the original detailed mechanism [23] and experimental data [24]. Nevertheless, the estimated mole fractions of other key species such as C$_2$H$_5$OH, O$_2$ and carbon monoxide (CO) for the optimised detailed mechanism at all $\phi$ are marginally affected by the adjusted Arrhenius rate constants, as seen in Figure 1(b), (c), (e), (f), (h) and (i). Conversely, the ID periods predicted by the optimised detailed mechanism at the initial pressures of 10.0 bar, 30.0 bar and 50.0 bar and with $\phi$ of 1.0 are more comparable to the experimental measurements [31] than those of the original detailed mechanism [23], as seen in Figure 2.

\[
\text{Normalised individual temperature sensitivity coefficient} = \frac{\text{Absolute individual temperature sensitivity coefficient}}{\text{Maximum individual temperature sensitivity coefficient}}
\] (1)
Here, the capability of the reduced mechanism in predicting the auto-ignition process was selected as the basis of reduction, an approach which is similar to the authors’ previous work [22]. Since the detailed mechanism for ethanol contained only 57 species and 383 reactions where the relations among the species are strong [32,33], mathematical reduction techniques such as directed relation graph (DRG) [34,35] which are more suitable for mechanisms with large groups of isomers [35] were thus not adopted. Therefore, unimportant reactions in the optimised detailed mechanism for ethanol [23] were removed based on the aforementioned temperature sensitivity analysis, whereby the sensitivities for all elementary reactions with respect to the pre-exponential factors (A-factors) in the Arrhenius reaction rate equations were calculated using CHEMKIN-Pro [22]. Before removing the unimportant reactions in the optimised detailed mechanism, the major reaction pathway in the detailed mechanism for ethanol was identified, as illustrated in Figure 3. Furthermore, species related to fuel ($\text{C}_2\text{H}_5\text{OH}$), oxidisers ($\text{O}_2$, hydroperoxyl ($\text{HO}_2$) and hydroxyl (OH)) and soot ($\text{C}_2\text{H}_2$, $\text{C}_2\text{H}_4$ and ethane ($\text{C}_2\text{H}_6$)) were set as the target species during the reduction process. This was to ensure that the chemical comprehensiveness of the detailed mechanism was retained in the reduced mechanism [22]. For the temperature sensitivity analysis, the absolute temperature sensitivity coefficient for an individual reaction was taken at the point of ignition for all initial temperatures from 750 K to 1350 K [22]. Reactions with normalised sensitivity coefficient values calculated using Equation 1 which were lower than a user-defined threshold, $\varepsilon_{\text{sd}}$, were deemed unimportant and thus eliminated. As a result, a reduced chemical kinetic mechanism for ethanol with 37 species and 149 reactions was developed.

2.2 Validation of the reduced chemical kinetic mechanism for ethanol under auto-ignition and JSR conditions
The reduced mechanism formulated for ethanol with 37 species and 149 reactions was validated by comparing the predicted ID periods against experimental measurements [31] and also the detailed mechanism predictions using the zero-dimensional (0D) closed homogenous reactor model in CHEMKIN-Pro. Table 1 shows the initial conditions defined for the 0D closed homogenous reactor. The ID period which is an important parameter to describe the auto-ignition phenomena was defined as the time when the initial temperature of an air-fuel mixture increases by 400 K [27]. During the reduction process, the ID periods for ethanol predicted by the reduced mechanism were constantly compared to those of the detailed mechanism to ensure that the ID periods of the reduced mechanism did not deviate more than 30% [35]. As presented in Figure 4(a) to (c), the ID predictions of the reduced mechanism were not more than 8.6% different from those of the detailed mechanism. Meanwhile, the measured ID periods at the initial pressures of 10.0 bar, 30.0 bar and 50.0 bar and $\phi$ of 1.0 were reproduced by the 37-species reduced mechanism within a maximum deviation of 0.5 order. This deviation is identical to that found between the detailed mechanism predictions and experimental data [31]. Furthermore, the ID periods predicted by the reduced mechanism at the initial pressures of 40.0 bar and 60.0 bar and $\phi$ between 0.5 and 1.5 were compared to those of the detailed mechanism. The reason the initial pressures of 40.0 bar and 60.0 bar were chosen was to emulate the typical ambient pressures in a diesel engine at the start of main injection [22]. Based on Figure 5(a) and (b), a good level of agreement is achieved for the ID periods predicted using both the reduced and the detailed mechanisms at the initial pressures of 40.0 bar and 60.0 bar and $\phi$ from 0.5 to 1.5, where a maximum deviation of 11.1% is found.

Furthermore, the steady-state extinction process for ethanol was modelled using the 0D perfectly stirred reactor (PSR) model in CHEMKIN-Pro. The 37-species reduced mechanism was validated by comparing the mole fractions of key species calculated using the reduced mechanism for air-ethanol mixtures diluted with nitrogen against the experimental data [24].
and also detailed mechanism predictions. Identical initial conditions to those of the JSR experiment carried out by Leplat et al. [24] were used here, as shown in Table 1. The mole fractions of selected species such as reactants (C₂H₅OH, O₂), oxygenated products (CO, carbon dioxide (CO₂)) and also species related to soot formation (C₂H₄ and C₂H₆) were of interest here, as illustrated in Figure 6(a) to (i). This was to ensure the fuel oxidation and soot formation/oxidation for ethanol fuel was adequately represented by the 37-species reduced mechanism. Based on Figure 6(a) to (i), the mole fractions of C₂H₅OH, O₂, CO, CO₂ and C₂H₆ were reasonably reproduced by the reduced mechanism when compared to those of the detailed mechanism and experimental measurements [24]. Meanwhile, the peak C₂H₄ mole fraction of the reduced mechanism at \( \phi \) of 0.6 is decreased by 40% as compared to the experimental data [24], as seen in Figure 6(c). In addition, the location of peak C₂H₄ mole fraction for the reduced mechanism is shifted to 1050 K while that of the experiment is at 900 K. Nevertheless, a good consistency is obtained for the predicted C₂H₄ mole fractions between the reduced and detailed mechanisms. These results in-turn demonstrate the capability of the 37-species reduced mechanism formulated for ethanol.

2.3 Formulation of the reduced mechanism for SME-ethanol

The reduced mechanism for biodiesel-ethanol was formulated using a similar approach to that reported by Ng et al. [36], where the reduced mechanism for biodiesel [22] was used as the base mechanism. Common reactions in the reduced mechanism for ethanol were replaced by those in the reduced biodiesel mechanism [22]. Meanwhile, the associated reactions which were unique to ethanol in relative to biodiesel were added into the reduced mechanism for biodiesel-ethanol. Apart from that, the non-unique thermodynamic data for ethanol were revised to those of the biodiesel. As a result, a reduced mechanism for biodiesel-ethanol with
102 species and 446 reactions was formulated. Figures 4 and 5 plot the ID periods predicted using the ethanol sub-mechanism of the biodiesel-ethanol surrogate mechanism against those of the detailed mechanism [23] and 37-species reduced mechanism for ethanol, at the initial pressures between 10.0 bar and 60.0 bar. Overall, a good agreement is obtained when comparing the ID periods, whereby 86% of the predictions by the ethanol sub-mechanism of the biodiesel-ethanol surrogate mechanism fall within a deviation range of 20% to 30%. As such, the Arrhenius rate constants for the ethanol sub-mechanism of the biodiesel-ethanol mechanism were not further adjusted to prevent over-optimisation. Additionally, the predictions of the ethanol sub-mechanism were also compared against the experimental measurements [24] and the detailed mechanism predictions, under the JSR conditions. As seen in Figure 6, the mole fractions of C$_2$H$_5$OH, CO, CO$_2$, C$_2$H$_4$, C$_2$H$_6$ and O$_2$ predicted using the ethanol sub-mechanism were comparable to those of the detailed mechanism and experimental measurements. Thus, this demonstrates the reasonable predictability of the combined surrogate mechanism for the biodiesel-ethanol blend in spite of the revised thermodynamic data.

3. Modelling of spray combustion for SME and SME-ethanol blends

3.1 Formulation of spray combustion simulations

In this reported work, the Sandia Spray A experiment conducted by Nerva et al. [37] for SME fuel was selected for modelling the spray combustion processes. SME fuel was injected at an injection pressure of 1500 bar into a cubical constant volume combustion chamber with equivalent edges of 108 mm. The operating conditions replicated those of the diesel engine, at a constant ambient density of 22.8 kg/m$^3$ and ambient temperatures of 900 K and 1000 K. Table 2 lists the full operating conditions of the experimental setup.
The validation of the spray combustion simulations was conducted by comparing the liquid penetration lengths (LPL), vapour penetration lengths predicted for SME against the experimental measurements [37], under the non-reacting spray condition [38]. In order to reduce the computational runtime, a 4° two-dimensional (2D) axisymmetric computational mesh was used to simulate the combustion processes in OpenFOAM. This approach was adopted from Pei et al. [39] and Pang et al. [40], where the total volume of the 2D axisymmetric computational mesh was calibrated to be equivalent to the experimental constant volume combustion chamber. As such, the axial length of the 2D axisymmetric computational mesh was adjusted to 138.0 mm while the radial length was set at 54.0 mm, as illustrated in Figure 7. Meanwhile, the fixed wall and wedge boundary conditions were applied on the lateral sides of the computational mesh, as indicated in Figure 7. Both the spatial and temporal resolutions were subsequently examined. As shown in Figure 8(a), (b), (d) and (e), mesh independence was achieved when the initial cell sizes in the axial and radial directions were set to 0.50 mm and 0.25 mm, respectively. This in-turn led to the formation of 10,816 cells for the 2D axisymmetric computational mesh. Meanwhile, Figure 8(c) and (f) depict that converged solutions were obtained when the time-step size was fixed at 0.5 μs as further reduction in the time-step size to 0.1 μs did not improve the accuracy of the numerical results [38].

Table 2 tabulates the CFD models and baseline model constants specified for the spray combustion simulations. The combined biodiesel-ethanol mechanism of 102 species and 446 reactions for the SME and SME-ethanol fuels were embedded directly into OpenFOAM version 2.0.x. The chemical kinetics was solved using the well-stirred reactor approach in which the effects of sub-grid turbulence chemistry interactions were excluded. In order to reproduce the secondary spray breakup, the Reitz-Diwakar spray breakup model [41] was implemented, for which the stripping breakup time constant ($C_s$) for SME was calibrated to 15.0 [38]. Meanwhile, the Reynolds Averaged Navier-Stokes (RANS) method was used to
simulate the turbulent flow. The standard $k$-$\varepsilon$ model was applied here and the turbulent model constant ($C_1$) value was adjusted to 1.59 based on its approximation of round jets [42]. The initial turbulence kinetic energy ($k$) and initial turbulence dissipation rate ($\varepsilon$) were set to 0.735 $\text{m}^2/\text{s}^2$ and 3.835 $\text{m}^2/\text{s}^3$, respectively [22]. The Leung and Lindstedt multi-step soot model [43] was used to calculate soot formation with $\text{C}_2\text{H}_2$ set as the soot precursor. Both OH and O$_2$ were considered in the Fenimore and Jones model [44] as the primary oxidising agents to calculate the soot oxidation.

Figure 9 presents the significant thermo-physical properties which included liquid density, liquid surface tension, vapour pressure and latent heat of vaporisation for the SME and ethanol fuels over a temperature range of 280 K up till the critical temperature of the respective fuels. The thermo-physical properties reported in the authors’ previous work [38] were used for SME while those for ethanol were adopted from the library of thermo-physical properties in OpenFOAM version 2.0.x. The liquid surface tension for ethanol in OpenFOAM version 2.0.x was revised according to that in OpenFOAM version 1712 due to a discrepancy.

The numerical case settings for spray combustion, excluding the fuel compositions as well as the associated thermo-physical properties and chemical kinetics, for the SME-ethanol blends were set identical to those of the SME fuel. This was also to ensure that only the effects from the fuel properties and chemical kinetics due to the fuel compositions were present in the numerical results produced for the SME-ethanol blends.

### 3.2 Predicted spray combustion characteristics for SME and SME-ethanol blends

Since alcohols exhibit low cetane numbers, in this case ethanol has a cetane number of 8 as shown in Table 3, only small concentrations of alcohol fuels are recommended for use in existing diesel engine setups [13] as physical engine modification is required when high levels
of alcohol fuels are used. Meanwhile, based on the preliminary simulation results for SME-ethanol blends from S90E10 to S50E50 (with a blend interval of 10% by vol.), the effects of the 10% blend interval on the spray combustion predictions for the SME-ethanol fuels were less discernible as compared to a 20% (by vol.) blend interval. As such, two different SME-ethanol blends, namely 90%-10% (by vol.) of SME-ethanol (S90E10) and 70%-30% (by vol.) of SME-ethanol (S70E30) are examined in this work.

Table 4 shows the predictions of averaged LPL, ID periods and FLLs for SME and SME-ethanol blends at the ambient temperatures of 900 K and 1000 K. When compared to those of the SME, the LPLs predicted for S90E10 at both 900 K and 1000 K are reduced by maximum deviations of 23.5% and 22.9%, respectively. As the ethanol content increases to 30%, the predicted LPLs at 900 K and 1000 K are further shortened by 35.5% and 25.5%, respectively as compared to those of the SME. Here, it is worth to highlight that the effects of the increased ethanol content in the SME-ethanol blends are only prominent at 900 K while those at 1000 K are considered marginal since the LPLs for S90E10 and S70E30 are similar. These results are in agreement to that obtained by Li et al. [45], where a shorter spray penetration was found for the diesel-n-butanol blend compared to that of the diesel fuel at ambient pressures of 10.0 bar to 20.0 bar and an ambient temperature of 288 K. The reduction in LPLs observed for S90E10 and S70E30 may be attributed to the differences in the thermo-physical properties for SME fuel and SME-ethanol blends. Based on Table 3, it is found that the measured physicochemical properties such as density, kinematic viscosity and lower heating value for the ethanol fuel are less than those of the SME fuel. Additionally, among the significant individual thermo-physical as identified previously [38], ethanol has lower liquid density and liquid surface tension, but higher vapour pressure and latent heat of vaporisation in comparison to those of the SME as illustrated in Figure 9. These thermo-physical properties which are pertinent to the spray penetration [38,46] indicate lower momentum [47] and higher
fuel evaporation rate [48]. This subsequently reduces the spray penetration of the SME-ethanol blends across the combustion chamber.

Here, the ID period is set as the duration when the maximum flame temperature first reaches 2000 K [49]. As seen in Table 4, the ID periods calculated for the SME-ethanol blends at both the ambient temperatures of 900 K and 1000 K are elongated in accordance to the increase in ethanol content of the SME-ethanol blends. Small elongations of 3.3% and 5.0% are found when the ID periods calculated for S70E30 at the ambient temperatures of 900 K and 1000 K are compared to those of SME, respectively. Despite this, these results demonstrate similar trends to those in the literature whereby the ID periods for biodiesel-ethanol blends are longer [18,21,50]. Apart from that, the trends are similar to those obtained under the 0D auto-ignition conditions as shown in Figure 10. As compared to those of the SME, the ID periods predicted for S90E10 and S70E30 at the initial pressure of 60.0 bar and around the negative temperature coefficient region (between temperatures of 850 K and 1050 K) are elongated by maximum deviations of 28.5% and 34.4%, respectively. The delay in the ID periods with respect to the increase in ethanol content of the SME-ethanol blends corresponds to the cetane numbers of the fuels, where the cetane number measured for ethanol is 85% lower than that of the SME (Table 3).

In order to further examine the auto-ignition behaviours for SME and SME-ethanol blends, temporal distributions of $\phi$, which was defined according to that by Jangi et al. [51], against the local flame temperatures ($T$) are plotted. The $\phi$-$T$ distributions at both the ambient temperatures of 900 K and 1000 K indicate the spray and flame developments for SME and SME-ethanol blends at the point of ignition and quasi-steady state as seen in Figure 11(a) to (f). At 0.4 ms, the $\phi$-$T$ distributions for S90E10 and S70E30 at 900 K are slightly smaller as compared to that of the SME as shown in Figure 11(a). These distributions continue till the ignition point of each fuel. Based on Figure 11(c), the $\phi$-$T$ distribution for SME is the largest
as compared to those of the S90E10 and S70E30. Meanwhile, the $\phi$-$T$ areas for the S90E10 and S70E30 are reduced when the ethanol content increases from 10\% to 30\%. Here, some mixtures of SME are located at higher $\phi$, up till approximately 4.3, whilst those of the S90E10 and S70E30 are found at maximum $\phi$ values of 3.0 and 3.3, respectively. Nevertheless, the mixtures of SME and SME-ethanol blends similarly ignite around the lean side of the stoichiometric line which is between $\phi$ of 0.9 and 0.95 as found in Figure 11(c).

Adopting the conceptual framework of quasi-steady combustion for diesel [52], the rich pre-mixed core and outer diffusion flame are labelled on the quasi-steady $\phi$-$T$ distributions (at approximately 1.5 ms) for SME, S90E10 and also S70E30 at both 900 K and 1000 K as illustrated in Figure 11(e) and (f). Here, the classic non-premixed turbulent flame structure [52] is observed for SME, S90E10 and also S70E30. The maximum flame temperatures for SME, S90E10 and S70E30 are also identically located on the lean side of flame, at $\phi$ of 0.9. However, an increase of 60 K is found when comparing the predicted maximum flame temperature for S70E30 against that of the SME. The flame areas in terms of width predicted for S90E10 and S70E30 are also reduced whereby the regions of rich pre-mixed core for both fuels are located at a range of $\phi$ less than that of the SME.

Despite the increase in ambient temperature, Figure 11(b), (d) and (f) show that the spray/flame evolutions calculated for SME, S90E10 and S70E30 at 1000 K display a similar behaviour to that at 900 K. The $\phi$-$T$ distributions predicted at 0.4 ms and the ignition points reduce in response to the increase in ethanol content of the SME-ethanol blends, where that of the S70E30 is the smallest as can be seen in Figure 11(b) and (d). Additionally, the increase in ethanol also leads to a decrease in the $\phi$ values at which the regions of the diffusion flames for S90E10 and S70E30 are located as presented in Figure 11(f). Although the maximum flame temperatures for SME, S90E10 and S70E30 at the quasi-steady state (1.5 ms) are located at rather similar $\phi$ values between 0.81 and 0.83, the magnitude of maximum flame temperature
for S70E30 is about 30 K higher than that of SME. This is line with the trend estimated at 900 K. It is also noteworthy to mention that the locations of maximum flame temperatures for SME and SME-ethanol blends are leaner than that observed for n-dodecane spray flame at identical tested conditions [53]. This is because Bhattacharjee and Haworth [53] defined the ID period as the interval from the start of injection till the local flame temperature exceeded 400 K of the ambient temperature.

FLL is defined as the axial distance between the injector and the first position where 2.0% of Favre-averaged OH mass fractions is found [22]. As shown in Table 4, the FLLs calculated for the SME-ethanol blends did not vary with respect to the increase in ethanol content where the FLLs estimated for S90E10 and S70E30 at both ambient temperatures of 900 K and 1000 K are similar to those of the SME. Since FLL indicates the combustion behaviours [54], the FLL predictions here are in agreement with the predicted classic non-premixed turbulent flame structures seen in Figure 11(e) and (f), where both the FLLs and non-premixed flames for S90E10 and S70E30 at 900 K and 1000 K are similar to those of the SME. Furthermore, the similarity in the FLL predictions among the tested fuels are also indicated by the OH mass fractions at the quasi steady-state, for which the distributions and the location of peak OH mass fractions for the S90E10 and S70E30 fuels are similar to those of the SME fuel as shown in Figure 13(a) and (b). However, these results are in contrast to the fuel reactivity denoted by the fuel cetane number [55], where FLL elongates as the fuel reactivity is reduced. Ethanol which has a lower fuel reactivity than SME as indicated by its smaller fuel cetane number may contribute to a further spray lift-off when it is blended with SME. Nevertheless, the trend observed for the FLL predictions here is not uncommon as it has been reported that the FLLs for various diesel [56] and biodiesel [54] fuels did not correspond to the change in the cetane number and volatility of diesel [56] and biodiesel [54] fuels. Apart from that, Persson et al. [57] and Moon et al. [58] highlighted that the FLLs were also dependent on the
combination of fuel types, injection conditions and ambient conditions. As such, the effects of the increase in ethanol content of the SME-ethanol blends on the FLL predictions are insignificant.

3.3 Predicted soot characteristics for SME and SME-ethanol blends

The predicted quasi-steady \( \text{C}_2\text{H}_2 \) mass fractions, soot volume fractions (SVFs) and rates of soot surface growth against \( \phi \) for SME and SME-ethanol blends at the ambient temperatures of 900 K and 1000 K are presented in Figure 12. As the ethanol percentage in the SME-ethanol blends increases to 30%, a reduction of approximately 19.6% in the peak SVF at 900 K is found. This is in agreement with the findings obtained by Shudo et al. [18] and Moon et al. [58] for PME-ethanol and diesel-ethanol blends, respectively. The lower SVF\(\phi\)s found for the SME-ethanol blends are associated with the reduced \( \text{C}_2\text{H}_2 \) mass fractions. As seen in Figure 12(a), the peak \( \text{C}_2\text{H}_2 \) mass fraction calculated for S70E30 is 10% less than that of SME. In addition, the reduction in SVFs for the SME-ethanol blends at 900 K is also attributed to the lower soot surface growth rates. When comparing the predicted maximum soot surface growth rates for S70E30 against those of the SME, a maximum decrease of 20% is obtained as illustrated in Figure 12(e). Similarly, these trends are observed at the ambient temperature of 1000 K for which the predicted peak values of SVF for S90E10 and S70E30 are relatively less than those of the SME fuel by 3.8% and 12.6%, respectively as depicted in Figure 12(d). These reductions are attributed to the both decreases of approximately 6% in the mass fractions of \( \text{C}_2\text{H}_2 \), which was set as the soot precursor, and also 11% in the subsequent rates of soot surface growth estimated for S90E10 and S70E30 as displayed in Figure 12(b) and (f), respectively. Apart from that, the decrease in the SVFs for S70E30 and S90E10 is also contributed by the OH
group in ethanol which suppresses soot formation [59,60] while the additional double bonds in SME have higher tendencies to form unsaturated species i.e. $\text{C}_2\text{H}_2$ [61].

Figure 13 shows the calculated quasi-steady mass fractions of OH and $\text{O}_2$ as well as the rates of soot oxidation due to OH and $\text{O}_2$ for SME, S90E10 and S70E30 at the ambient temperatures of 900 K and 1000 K. It is found that the effect of the increase in ethanol percentage of the SME-ethanol fuels is marginal on the overall calculated mass fractions of OH and $\text{O}_2$ at both ambient temperatures as illustrated in Figure 13(a) to (d). According to Figure 13(a) and (b), the predicted distributions of OH mass fractions for S90E10 and S70E30 are identical to those of the SME fuel at 900 K and 1000 K. The peak OH mass fractions for the SME and SME-ethanol fuels are situated at identical $\phi$, approximately between 0.77 and 0.80. Similar prediction is also found for the $\text{O}_2$ mass fractions, as illustrated in Figure 13(c) and (d). While the distributions of $\text{O}_2$ mass fractions for S90E10 and S70E30 are slightly smaller than those of SME, the locations of peak maximum $\text{O}_2$ mass fractions for the SME and SME-ethanol fuels are found at a $\phi$ of 0.29. This may be a result of the dominance of the ambient $\text{O}_2$ level where the maximum $\text{O}_2$ mass fractions at both 900 K and 1000 K are recorded at 15% (by vol.) despite the change in fuel types.

However, these results do not indicate that the rates of soot oxidation due to OH and $\text{O}_2$ which are typically found at $\phi$ values between 1 and 2 do not vary with respect to the increase in ethanol content of the SME-ethanol fuels. As displayed in Figure 13(e) and (f), the peak rates of soot oxidation due to OH for S90E10 and S70E30 at both 900 K and 1000 K are reduced by a maximum deviation of 15.2%, as compared to those of the SME. Meanwhile, the peak soot oxidation rates due to $\text{O}_2$ predicted for S70E30 at both 900 K and 1000 K are less than those of the SME by a maximum difference of 10.5% as seen in Figure 13(g) and (h), respectively. However, the soot oxidation rates due to $\text{O}_2$ for S90E10 at both 900 K and 1000 K are comparable to those of the SME as shown in Figure 13(g) and (h). This denotes that the
effect of ethanol on the soot oxidation rates due to O\textsubscript{2} for the SME-ethanol blends is only noticeable when the ethanol percentage in the SME-ethanol blend is high.

### 3.4 Rate of production (ROP) analyses

The predictions of SVF and also rates of soot surface growth for SME and SME-ethanol blends are further justified by the ROP analyses in CHEMKIN-Pro, where C\textsubscript{2}H\textsubscript{2} was set as the target species. The ROPs for C\textsubscript{2}H\textsubscript{2} were analysed at an initial pressure of 60.0 bar, ambient temperatures of 900 K and 1000 K and \(\phi\) of 1.5. A \(\phi\) value of 1.5 was set here is because this is the region at which the highest SVFs for SME and SME-ethanol blends are found as seen in Figure 12(c) and (d).

The absolute C\textsubscript{2}H\textsubscript{2} ROPs for SME, S90E10 and S70E30 as illustrated in Figure 14 are obtained at a temperature of 2000 K. The positive and negative signs of the ROP values on the horizontal axes of Figure 14(a) and (b) denote forward and backward reactions, respectively. Although the reactions to form C\textsubscript{2}H\textsubscript{2} for SME and SME-ethanol blends are identical as seen in Figure 14(a) and (b), the absolute ROP values are different. The individual C\textsubscript{2}H\textsubscript{2} ROP at 900 K and \(\phi\) of 1.5 for S90E10 and S70E30 are 17.4\% lower than those of the SME, as seen in Figure 14(a). The C\textsubscript{2}H\textsubscript{2} ROP analyses at 1000 K demonstrate identical trends to those at 900 K, where the ROP values for S90E10 and S70E30 are less than those of the SME but with a smaller decrease of 5\%, as shown in Figure 14(b). Here, the ROP predictions are in line with the discussion in Section 3.3 in which the C\textsubscript{2}H\textsubscript{2} mass fraction for SME-ethanol blends are lower. As a result, decreases in the soot surface growth rates and also the subsequent SVFs are found for S90E10 and S70E30.

### 4. Conclusions
In this reported work, the effects of ethanol addition on the spray combustion and soot formation/oxidation of SME-ethanol blends were elucidated and compared against those of the SME. At the ambient temperatures of 900 K and 1000 K, a maximum reduction of 35.5% in the LPLs was obtained for S90E10 and S70E30. The ID periods for the SME-ethanol blends were delayed by only 5.0%. Meanwhile, the FLLs predicted for both the S90E10 and S70E30 did not change in comparisons to those of the SME at 900 K and 1000 K. This was in line with the predicted classic non-premixed turbulent flame structures obtained for SME, S90E10 and also S70E30. During the quasi-steady state at 900 K and 1000 K, smaller distributions of spray/flame development and with a higher local flame temperature of 60 K (maximum difference) were found for the SME-ethanol blends. Despite these, the SVFs predicted for S90E10 and S70E30 were reduced according to the increase in ethanol content of the SME-ethanol blends. The maximum SVFs estimated for S90E10 and S70E30 at 900 K were decreased by 10.2% and 19.6%, respectively. Similar trends were also found at 1000 K, for which the SVFs for the SME-ethanol blends were lower by a maximum difference of 12.6%. The reduction in SVFs obtained for S90E10 and S70E30 were collectively contributed by the decrease in both the soot surface growth rates and C₂H₂ mass fractions. These are further justified by the ROP analyses, where the mass fractions of C₂H₂ predicted for the SME-ethanol blends at 900 K and 1000 K were reduced by 17.4% and 5.0%, respectively when compared to those of the SME. In addition, the increase in ethanol content also led to a maximum decrease of 15.2% in the peak rates of soot oxidation due to OH and O₂ predicted for the SME-ethanol blends. Based on these results, it can be concluded that only the LPL, spray/flame distributions, SVFs and soot formation/oxidation rates vary according to the increase in ethanol content of the SME-ethanol blends. However, changes in the aforementioned results are only discernible when the ethanol content in the biodiesel-ethanol blends is high i.e. S70E30.
References


[42] Novella R, García A, Pastor JM, Domenech V. The role of detailed chemical kinetics on


Table 1 Initial conditions specified for the 0D simulations in closed homogenous reactor and PSR.

<table>
<thead>
<tr>
<th>Operating condition</th>
<th>Parameter</th>
<th>Range evaluated</th>
</tr>
</thead>
<tbody>
<tr>
<td>Auto-ignition(^a)</td>
<td>Initial pressure (bar)</td>
<td>10.0, 30.0, 50.0</td>
</tr>
<tr>
<td></td>
<td>Initial temperature (K)</td>
<td>800 – 1300 (increment of 100 K)</td>
</tr>
<tr>
<td></td>
<td>(\phi) (-)</td>
<td>1.0</td>
</tr>
<tr>
<td>Auto-ignition(^b)</td>
<td>Initial pressure (bar)</td>
<td>40.0(^b), 60.0(^b)</td>
</tr>
<tr>
<td></td>
<td>Initial temperature (K)</td>
<td>750 – 1350 (increment of 100 K)</td>
</tr>
<tr>
<td></td>
<td>(\phi) (-)</td>
<td>0.5, 1.0, 1.5</td>
</tr>
<tr>
<td>JSR(^c)</td>
<td>Initial pressure (bar)</td>
<td>10.1</td>
</tr>
<tr>
<td></td>
<td>(\phi) (-)</td>
<td>0.6, 1.0, 2.0</td>
</tr>
<tr>
<td></td>
<td>Residence time (s)</td>
<td>0.7</td>
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</table>

\(^a\) Conditions defined based on the experiment conducted by Cancino et al. [31].

\(^b\) Conditions defined based on typical in-cylinder pressure values during main fuel injection event for light-duty, direct injection diesel engines [62].

\(^c\) Conditions defined based on the experiment conducted by Leplat et al. [24].
Table 2 Operating conditions and numerical settings for the spray combustion, adapted from Cheng et al. [38].

<table>
<thead>
<tr>
<th>Ambient conditions</th>
<th>Initial values</th>
<th>Boundary conditions</th>
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<tbody>
<tr>
<td>Temperature (K)</td>
<td>900, 1000</td>
<td>Zero-gradient</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>6.0, 6.7</td>
<td>Zero-gradient</td>
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<tr>
<td>Density (kg/m$^3$)</td>
<td>22.8</td>
<td>-</td>
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<tr>
<td>$k$ (m$^2$/s$^2$)</td>
<td>0.735</td>
<td>Standard wall function</td>
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<tr>
<td>$\varepsilon$ (m$^2$/s$^3$)</td>
<td>3.835</td>
<td>Logarithmic law-of-the-wall</td>
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<td>Air compositions (-)</td>
<td>N$_2$: 0.7515</td>
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</tr>
<tr>
<td></td>
<td>O$_2$: 0.15</td>
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<tr>
<td></td>
<td>H$_2$O: 0.0362</td>
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</tr>
<tr>
<td></td>
<td>CO$_2$: 0.0623</td>
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**Injection settings**

<table>
<thead>
<tr>
<th>Duration (ms)</th>
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<tbody>
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<td>Nozzle diameter (μm)</td>
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</table>

**Numerical settings**

<table>
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<th>Grid (mm)</th>
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<tr>
<td>Time-step size (μs)</td>
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<tr>
<td>Spray model</td>
<td>Reitz-Diwakar [41]; $C_s = 15$</td>
</tr>
<tr>
<td>Turbulence model</td>
<td>RANS standard $k$-$\varepsilon$; $C_l = 1.59$</td>
</tr>
<tr>
<td>Soot model</td>
<td>Formation: Leung and Lindstedt multi-step [43]; Oxidation: Fenimore and Jones [44]</td>
</tr>
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</table>
Table 3 Measured physicochemical properties for SME and ethanol.

<table>
<thead>
<tr>
<th>Physicochemical properties</th>
<th>SME(^a)</th>
<th>Ethanol(^a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemical formula</td>
<td>CH(_3)OOCR</td>
<td>C(_2)H(_5)OH</td>
</tr>
<tr>
<td>Molecular weight (kg/kmol)</td>
<td>292.6(^b)</td>
<td>46</td>
</tr>
<tr>
<td>Kinematic viscosity at 40°C (mm(^2)/s)</td>
<td>4.0</td>
<td>1.1</td>
</tr>
<tr>
<td>Density at 20°C (kg/m(^3))</td>
<td>887</td>
<td>790</td>
</tr>
<tr>
<td>Boiling point (°C)</td>
<td>342</td>
<td>78.4</td>
</tr>
<tr>
<td>Cetane number (-)</td>
<td>51</td>
<td>8</td>
</tr>
<tr>
<td>Lower heating value (MJ/kg)</td>
<td>37.53</td>
<td>26.8</td>
</tr>
</tbody>
</table>

\(^a\) Adapted from Liu et al. [63].

\(^b\) Approximated based on the fuel composition for fatty acid methyl esters in SME [22].
Table 4 Predicted averaged LPLs, ID periods and FLLs for SME, S90E10 and S70E30 at the ambient temperatures of 900 K and 1000 K, with a constant ambient density of 22.8 kg/m$^3$.

<table>
<thead>
<tr>
<th>Ambient temperature (K)</th>
<th>Predictions</th>
<th>Fuels</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>SME</td>
</tr>
<tr>
<td>900</td>
<td>Averaged LPL (mm)</td>
<td>18.3</td>
</tr>
<tr>
<td></td>
<td>ID periods (ms)</td>
<td>0.66</td>
</tr>
<tr>
<td></td>
<td>FLL (mm)</td>
<td>30.8</td>
</tr>
<tr>
<td>1000</td>
<td>Averaged LPL (mm)</td>
<td>15.3</td>
</tr>
<tr>
<td></td>
<td>ID periods (ms)</td>
<td>0.51</td>
</tr>
<tr>
<td></td>
<td>FLL (mm)</td>
<td>23.7</td>
</tr>
</tbody>
</table>
Fig. 1 Predicted species mole fractions of C\textsubscript{2}H\textsubscript{4}, C\textsubscript{2}H\textsubscript{6}, C\textsubscript{2}H\textsubscript{5}OH, O\textsubscript{2}, CO and CO\textsubscript{2} for the original and optimised detailed mechanisms of ethanol against experimental measurements, under JSR conditions \cite{24}, with an initial pressure of 10.1 bar and φ of (a) to (c) 0.6, (d) to (f) 1.0 and (g) to (i) 2.0.
Fig. 2 Predicted ID periods for the detailed mechanism of ethanol, with original and optimised Arrhenius rate constants against experimental measurements [31], at initial pressures of 10.0 bar, 30.0 bar and 50.0 bar and $\varphi$ of 1.0.
Fig. 3 Major reaction pathway of ethanol oxidation.
Fig. 4 Predicted ID periods for the detailed mechanism, reduced mechanism and sub-mechanism of the combined biodiesel-ethanol mechanism of ethanol against experimental measurements [31] under auto-ignition conditions, at initial pressures of (a) 10.0 bar, (b) 30.0 bar and (c) 50.0 bar and with $\phi$ of 1.0.
Fig. 5 Predicted ID periods for the detailed mechanism, reduced mechanism and sub-mechanism of the combined biodiesel-ethanol mechanism of ethanol under auto-ignition conditions, at initial pressures of (a) 40.0 bar and (b) 60.0 bar and with $\phi$ of 0.5, 1.0 and 1.5.
Fig. 6 Predicted species mole fractions of $\text{C}_2\text{H}_4$, $\text{C}_2\text{H}_6$, $\text{C}_2\text{H}_5\text{OH}$, $\text{O}_2$, $\text{CO}$ and $\text{CO}_2$ for the detailed mechanism, reduced mechanism and sub-mechanism of ethanol against experimental measurements [24], under JSR conditions, at an initial pressure of 10.1 bar and with $\phi$ of (a) to (c) 0.6, (d) to (f) 1.0 and (g) to (i) 2.0.
Fig. 7 Cross section of the 4° 2D axisymmetric computational mesh for the constant volume combustion chamber, adapted from Cheng et al. [38].
The LPL predicted using 1.0 mm cell size becomes unstable beyond 2.0 ms.

Fig. 8 Predicted LPL and VPL using initial cell sizes of 0.25 mm, 0.50 mm and 1.0 mm in the directions of (a), (d) axial and (b), (e) radial and using (c), (f) time-step sizes of 1.0 μs, 0.5 μs and 0.1 μs against experimental data [37], under non-reacting spray conditions, adapted from Cheng et al. [38].
Fig. 9 Calculated thermo-physical properties for SME and ethanol, at temperatures of 280 K until critical temperature of each fuel (516.25 K and 789.21 K for SME and ethanol, respectively): (a) liquid density, (b) liquid surface tension, (c) vapour pressure and (d) latent heat of vaporisation, adapted from Cheng et al. [38].
Fig. 10 Predicted ID periods for SME, S90E10 and S70E30 under auto-ignition conditions, at initial pressures of 40.0 bar and 60.0 bar and with $\phi$ of (a) 0.5, (b) 1.0 and (c) 1.5.
Fig. 11 Predicted $\phi$-$T$ distributions for SME, S90E10 and S70E30 at 0.4 ms, ignition points and 1.5 ms (quasi-steady state), at ambient temperatures of (a), (c), (e) 900 K and (b), (d), (f) 1000 K.

The rich pre-mixed cores for S90E10 and S70E30 are located at smaller $\phi$ than that of SME.
Fig. 12 Predicted quasi-steady $C_2H_2$ mass fractions, SVFs and rates of soot surface growth against $\phi$ for SME, S90E10 and S70E30, at ambient temperatures of (a), (c), (e) 900 K and (b), (d), (f) 1000 K.
Fig. 13 Predicted quasi-steady mass fractions of OH and O$_2$, and rates of soot oxidation due to OH and O$_2$ against φ for SME, S90E10 and S70E30, at ambient temperatures of (a), (c), (e), (g) 900 K and (b), (d), (f), (h) 1000 K.
Fig. 14 Calculated absolute C$_2$H ROPs for SME, S90E10 and S70E30, at the ambient temperatures of (a) 900 K and (b) 1000 K, an initial pressure of 60.0 bar and with $\phi$ of 1.5.