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# **Development of a Reduced Biodiesel Surrogate Fuel Model for Multi-Dimensional Computational Fluid Dynamic Simulations**

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Abstract. This work reports the development of a reduced biodiesel surrogate fuel model for multi-dimensional Computational Fluid Dynamic simulations. The model is derived using an integrated kinetic mechanism reduction scheme and the final chemistry comprises only 83 species. The model is well validated in zero-dimensional chemical kinetic calculations under a wide range of auto-ignition and jet-stirred reactor conditions. The fidelity of the model is also further assessed in two-dimensional simulations of a constant-volume combustion vessel with respect to the experimental results of soy-methyl ester combustion. The results obtained reveal that ignition delay, lift-off lengths and soot volume fractions are reasonably well replicated by the reduced model. Furthermore, the compositions of the reduced model are varied according to the saturation/unsaturation levels of various biodiesel feed-stocks, such as palm-methyl ester and sunflower-methyl ester. In this work, it is demonstrated that the reduced model can potentially be used as a universal surrogate fuel model to predict the reactivity of biodiesel feed-stocks with low degree of saturation ( $\leq$ 30%) in both kinetic and fuel spray simulations.

## 1. Introduction

In recent years, studies on alternative energy resources have actively progressed to pursue a solution for greenhouse gas emissions and depleting oil reserves. Among all, biodiesel has received significant attention worldwide as a cleaner alternative fuel to conventional diesel fuel owing to its great potential in reducing pollutant emissions. Biodiesel is a renewable energy source which can be produced locally from biological resources such as vegetable oils and animal fats. In comparison to the conventional diesel fuel, it contains higher amount of oxygen contents which facilitates the oxidations of soot precursors and results in reduced engine-out emissions [1]. Nonetheless, incomplete combustion may occur when vegetable oils with high viscosity and low cetane number are used, leading to lower engine power output. In view of this, better understanding of the fuel kinetics is essential. As chemical kinetics of the actual biodiesel fuel is highly complex, a compact yet comprehensive surrogate model is desired for cost-effective simulations. In the previous work [2], a 68-species surrogate model, namely MCBSv1, was derived based on the detailed model of Herbinet et al. [3]. The validation of MCBSv1 was limited to only ignition delay (ID) predictions in 0-D kinetic simulations. Despite the well-matched ID predictions, it was found that major species concentration profiles were not reproduced well. Hence, this paper aims to improve the model predictions of MCBSv1 under diesel engine-like conditions and to investigate the applicability of the revised model to serve as a generic model for biodiesel feed-stocks with different saturation levels in both 0-D and 2-D simulations.

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### 2. Development of revised biodiesel surrogate fuel

A wide range of JSR conditions is added as an additional data source for mechanism reduction on top of the auto-ignition conditions. The reduction procedure is performed using a five-stage chemical kinetic mechanism reduction scheme [4]. Here, the revised model is denoted as MCBSv2 for brevity. The nitrogen oxide (NO) sub-model derived from the GRI-MECH 2.11 is also integrated into the model to predict thermal NO formation. The MCBSv2 model is first validated in 0-D simulations using the operating conditions illustrated in Table 1(a). Closed homogeneous batch reactor and perfectly-stirred reactor (PSR) models of CHEMKIN-PRO software are applied. The compositions of MCBSv2 are determined based on the actual RME fuel shown in Table 1(c). Methyl decanoate (MD) and methyl-9-decenoate (MD9D) are selected to represent the saturated and unsaturated components of RME, respectively. The composition of n-heptane  $(n-C_7H_{16})$  is fixed at 50% (by mass) which is similar to the experimental study [5]. The remaining 50% of the fuel compositions is then divided based on the actual saturated/unsaturated compositions of RME. The final reduced MCBSv2 model consists of 83 species with 264 elementary reactions. The reduction process has contributed to ~97.5% reduction in the total number of species and reactions as compared to those of the detailed model.

(a) 0-D Simulations				(b) 2-D Simulations				
Auto	Φ(-)	0.5, 1.0, 2.0		$T_a(K)$		900/1000		
<u>Auto-</u> ignition	P (bar)	40, 60, 80		$\rho_a (kg/m^3)$		22.8		
	T (K)	650 - 1350		P <sub>a</sub> (MPa)		6/6.7		
	Φ(-)	0.5, 1.0, 2.0		t <sub>inj</sub> (ms)		7		
<u>JSR</u>	P (bar)	40, 60, 80		Ambient compositions:				
	$t_R(s)$	1		(i) reacting		$O_2: CO_2: H_2O: N_2 = 15\% : 6.23\% : 3.62\% : 75.15$		% : 3.62% : 75.15%
	Φ(-)	1.5		_			(in mole)	
<u>JSR</u>	P (atm)	1		(ii) non-reacting		$O_2: CO_2: H_2O: N_2 = 0\%: 6.52\%: 3.77\%: 89.71\%$		
	$t_R(s)$	0.1				(in mole)		
(c)	Actual fuel composi			tions		MCBSv1	& MCBSv2 fuel com	positions
Fuels	Saturati	ion (%)	Unsat	uration (%)	MD	) (%)	MD9D (%)	n-C7H16 (%)
RME	~6			~94		3	47	50
SME	~12			~88	~88		44	50
SFME	~32			~68		16	34	50
PME	~48			~52		24	26	50

Table 1. Operating conditions for (a) 0-D and (b) 2-D simulations; (c) Fuel compositions by mass.

#### 3. Model validations in 0-D chemical kinetic simulations

The results calculated by MCBSv2 are compared with those of the detailed model throughout all the tested conditions in Figure 1. Here, only ID plots at the initial pressure of 60 bar are presented since the same ID pattern is obtained at initial pressures of 40 bar and 80 bar. For the same reason, only results of the species profiles at initial pressure of 60 bar and  $\Phi$  of 1 are demonstrated for auto-ignition and JSR conditions as similar temporal evolution trends in the results are observed for  $\Phi$  of 0.5 and 2.

The overall IDs computed by MCBSv1 and MCBSv2 agree reasonably well with those computed by the detailed model, as shown in Figure 1(a). However, results in Figure 1(b) show that MCBSv2 yields better predictions in species profiles as compared to MCBSv1, especially at steady-state. The difference in the onset of formation/decomposition between the computed species profiles is due to the difference in ID calculated by the models. In Figure 1(c), the overall species trends computed by MCBSv2 for fuel oxidation under JSR conditions are in well agreement with the detailed model. However, noticeable deviations are observed between the predictions by MCBSv1 and the detailed model, with deviations of as high as one order of magnitude on the absolute values. The mole fractions of MD9D, n-C<sub>7</sub>H<sub>16</sub> and O<sub>2</sub> are over-predicted whereas CO and CO<sub>2</sub> are under-predicted throughout the tested temperature range. This is partly due to the elimination of important alkyl and alkyl- ester radicals during mechanism reduction procedure. The use of MCBSv2 successfully minimises the relative errors between the predictions by the reduced and detailed models to less than 40 %.

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**Figure 1.** (a) ID predictions (P=60 bar,  $\Phi=0.5$ , 1.0, 2.0); Species profiles of fuel oxidation under (b) auto-ignition and (c) JSR conditions; (d) Species mole fractions obtained from the oxidation of 0.05 % RME in a JSR. (Note: • experimental data,  $\circ$  detailed model,  $\cdots$  MCBSv1, - MCBSv2)

Further validations of the surrogate models are performed by comparing the computed species profiles to the experimental data [5] of RME oxidation in a JSR for fuel-oxygen mixtures, diluted by nitrogen. The results are shown in Figure 1(d). It is observed that the species mole fractions computed by MCBSv2 are comparable with those obtained from the experiments and the detailed model. Nonetheless, the computation results generated by MCBSv1 are seen to be relatively different from the measurements. Variations in species concentrations of  $CH_4$  and  $C_2H_4$  are more evident where both concentrations are under-predicted across the temperature range. As mentioned earlier, this can be attributed to the elimination of important alkyl and alkyl- ester radicals during the mechanism reduction procedure. As compared to MCBSv1, significant improvements in  $CH_4$  and  $C_2H_4$  concentrations are achieved with the use of MCBSv2, in which the computational results

are closer to the measured data. Despite the variations on absolute values, the species profiles predicted by MCBSv2 are consistent with those of the experiments and detailed model. The validation results are deemed acceptable in consideration of its simplified chemistry.

### 4. Model validations in 2-D spray combustion simulations

In this section, model validations of MCBSv2 in spray combustion phenomena are carried out using a spray combustion solver in OpenFOAM-2.0.x. The results are compared with the experimental measurements of SME fuel combustion in a constant volume combustion vessel [1], as shown in Figure 2. It is evident that the biodiesel feed-stock applied in the experiment is different from the target fuel (i.e. RME) applied in this study. However, this may be regarded as acceptable since the difference in the average saturated compositions between these two fuels is relatively small (~6%) and the experimental data available in the literature is also limited. The operating conditions applied in the simulations are illustrated in Table 1(b). Further details can be found in [4].



900 K (•) and 1000 K (•).

From Figure 2, it is observed that the predicted IDs and LOLs are evidently shorter than the measurements using MCBSv1. In contrast, improvements in the computational results are apparent with the use of MCBSv2. This can be attributed to the inclusion of the additional reaction pathways consisting important alkyl and alkyl-ester radicals during the model construction of MCBSv2. The overall ID predictions by the surrogate models are shorter than the measurements. This can be explained by the higher content of unsaturated compositions (i.e. MD9D) in RME, which promotes faster chain branching process owing to its location of double bond at the end of hydrocarbon chain. As a result of shorter IDs, the LOLs predicted for RME combustion are also shorter. Furthermore, qualitative comparisons of the predicted soot contours with respect to the experimental measurements at quasi-steady state (4ms after start of injection) are performed. The findings here show that MCBSv2 is able to provide better qualitative predictions of soot distributions in terms of soot location and soot length, as compared to MCBSv1. Apart from that, highest SVF is captured at the centre region of soot clouds for both cases. This corresponds with the fuel-rich region of the fuel jet.

## 5. Implementation of MCBSv2 as the generic surrogate model for various biodiesel feed-stocks

In this section, the applicability of MCBSv2 as a generic surrogate model for different biodiesel feedstocks, such as SME, SFME and PME, is examined. The compositions of MCBSv2 are adjusted based on those of the actual fuels, as shown in Table 1(c). Firstly, MCBSv2 is further validated using the JSR experimental results of methyl oleate/n-decane and methyl palmitate/n-decane oxidations carried out by Bax et al. [6] and Hakka et al. [7], respectively. The results are depicted in Figure 3. It is observed that the computations are close to the measurements for all three biodiesel feed-stocks. The predictions of MCBSv2 are also in fairly good agreement with those of the detailed counterpart for all three cases. Besides, it is seen that the overall  $CO_2$  productions computed by both the reduced and detailed models decrease with increment in the fuel saturation level. In contrast, an opposite trend is observed for  $C_2H_4$  and  $C_2H_6$ . These observations are consistent with the measured trends from the experiments [6]. It is noted that the biodiesel fuel blends applied in the simulations consist of a mixture of both saturated and unsaturated esters. On the contrary, the fuel blends used in the experiments only contain either saturated or unsaturated esters. Thus, the calculated results might be different from the measurements due to the presence of cross reactions between the saturated and unsaturated fatty acid methyl esters (FAME). It is concluded that overall agreements in temporal evolution trend between the experimental and computed species profile trends are achieved.



**Figure 3.** Species mole fractions obtained from the oxidation of (a) SME, (b) SFME and (c) PME in a JSR, with initial pressure of 106 kPa,  $\phi$  of 1.0 and  $t_R$  of 1.5 s. Horizontal dashed lines (--) indicate the maximum predicted species fraction among SME, SFME, and PME.

Next, the combustion characteristics and soot formation performances in response to the variation of fuel saturation level are examined with the use of MCBSv2. The operating conditions employed here can be found in Table 1(b) and results are shown in Figure 4. From Figure 4(a), it is observed that ID becomes longer when the fuel saturation level increases for both ambient temperatures. This can be explained by the higher amount of unsaturated FAME which promotes faster chain branching, leading to shorter ID and shorter flame lift-off. The findings here agree well with the computational results in the earlier 0-D kinetic simulations. Following that, the SVF predictions of RME, SME, SFME and PME along spray axis at quasi-steady state are depicted in Figure 4(b). It is observed that soot is formed at location nearest to the injector tip for RME combustion, followed by SME, SFME and PME for both 900 K and 1000 K cases. This can be attributed to the associated shorter LOLs. In addition, it is found that the predicted SVFs are the highest for RME combustion and lowest for PME combustion for both ambient temperatures. Among all the tested fuels, PME contains the lowest amount of unsaturated fatty acids and hence there are less double bonds in the fuel. It is reported that the

presence of double bonds in unsaturated FAME is the key reason for higher production of soot precursors and unsaturated hydrocarbons, which eventually leads to higher engine-out soot emission. This trend is well replicated by the model whereby SVF decreases with higher saturation level.



Figure 4. Simulated (a) ID, LOL and (b) SVF at ambient temperatures of 900 K and 1000 K.

# 6. Conclusions

MCBSv2 which is a revised model for rapeseed methyl ester with only 80 species is successfully formulated and validated in this study. Significant improvements in fuel reactivity predictions have been achieved with the use of MCBSv2 as compared to MCBSv1. The current findings suggest that MCBSv2 serves as a potential surrogate fuel model for biodiesel feed-stocks with low degrees of saturation ( $\leq$ 30%), such as the RME, SME and SFME, in both kinetic and spray simulations. The model accuracies in ignition delay and species profile predictions deteriorate rapidly when saturation level is greater than 30 %. Hence, further improvement is necessary such that it can be used as a surrogate model for highly saturated FAME, such as the coconut methyl ester which contains approximately 80 % of saturated esters in the fuel.

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