

Use of Detailed Kinetics and Advanced Chemistry-Solution Techniques in CFD to Investigate Dual-Fuel Engine Concepts

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ABSTRACT

A multi-component fuel model is used to represent gasoline in computational fluid dynamics (CFD) simulations of a dual-fuel engine that combines premixed gasoline injection with diesel direct injection. The simulations employ detailed-kinetics mechanisms for both the gasoline and diesel surrogate fuels, through use of an advanced and efficient chemistry solver. The objective of this work is to elucidate kinetics effects of dual-fuel usage in Reactivity Controlled Compression Ignition (RCCI) combustion. The model is applied to simulate recent experiments on highly efficient RCCI engines. These engine experiments used a dual-fuel RCCI strategy with port-fuel-injection of gasoline and early-cycle, multiple injections of diesel fuel with a conventional diesel injector [1]. The experiments showed that the US 2010 heavy-duty NO_x and soot emissions regulations were easily met without aftertreatment, while achieving greater than 50% net indicated thermal efficiency. However, as with other low-temperature combustion strategies, CO and unburnt hydrocarbon emissions must be controlled. Homogeneous charge compression ignition (HCCI) engine experiments were also earlier performed and simulated using a less detailed primary-reference-fuel (PRF) mechanism and single-component surrogates [1]. The present work introduces a more accurate multi-component representation of the gasoline and a more detailed kinetics mechanism for both the gasoline and diesel surrogates. The simulation results show accurate representation of combustion phasing and better predictions of unburned hydrocarbons and CO emissions as an outcome of using the detailed kinetics. The model demonstrates that

the most-reactive surrogate component, n-heptane (component in both diesel and gasoline) ignites first, and the other, slower gasoline-surrogate components follow. The model also shows that the slowest gasoline surrogate component, toluene, is found disproportionately in the unburned hydrocarbon (UHC) emissions. Overall, the predicted UHC emissions can be broadly classified into three groups: surrogate-fuel species make up 37 wt%, large hydrocarbon intermediates that form from the surrogate fuels form 42 wt%, and small C₁-C₄ hydrocarbons form 21 wt%. Of the surrogate fuels present, toluene has the largest concentration. Analysis of uncertainties in IVC temperature input on emissions predictions has also been performed. As the combustion phasing is retarded, the UHC and CO emissions increase for the base case and the uncertainties in temperature have a more dominant effect on emissions.

INTRODUCTION

Kokjohn et al. [1] recently proposed a Reactivity Controlled Compression Ignition (RCCI) combustion strategy. Engine experiments were conducted that used dual-fueling with port-fuel-injection of gasoline and early cycle multiple injections of diesel fuel with a conventional diesel injector. The experiments showed that the US 2010 heavy-duty NO_x and soot emissions regulations were easily met without aftertreatment, while achieving greater than 50% net indicated thermal efficiency.

The present work builds on the earlier modeling work of Kokjohn et al. [1], but uses a more realistic gasoline

surrogate, and a more detailed kinetics model for simulating both HCCI and RCCI engine conditions. As will be seen, this allows more accurate prediction of UHC and CO emissions, which are of interest in optimized engine combustion. In the sections below, we first describe the approach for formulating the fuel model, including comparison to simpler approaches. Next, we discuss the origin of the detailed kinetics mechanism used for the model-fuel blend, its validation history and the mechanism-reduction strategies employed. This is followed by discussion of the CFD model inputs and, finally, the HCCI and RCCI simulation results, with comparison to experimental data. The final section includes discussion of the insights gained from the detailed-kinetics representation of the fuels.

MODEL FUEL BLEND

The complexity of the model fuel needed to represent real fuels depends on the purpose of the simulation. More complex surrogates can better represent the chemical and physical properties of the fuel, but require larger chemistry mechanisms and hence higher computational cost. Simple one- and two-component surrogates, and relatively simple chemistries, have been used successfully to model conventional diesel engines; examples include the work of Ra et al. [2] and Golovitchev et al. [3]. HCCI and RCCI combustion, on the other hand, are much more sensitive to the chemistry of the fuel, and hence need more complex multi-component fuel surrogates to capture fuel reactivity accurately. Ideally, we would use multi-component surrogates to represent both gasoline and diesel in a dual-fuel engine. However, Kokjohn et al. [1] showed that the optimum gasoline/diesel fuel consisted mainly of gasoline (~70-85 wt %). Thus, the present study focused on expanding the representation of the gasoline, while keeping a simple one-component surrogate for the injected diesel.

DIESEL SURROGATE

A one-component surrogate was considered that consists of n-heptane for the chemical representation of the diesel fuel. However, we use the physical properties of n-tetradecane to represent the diesel spray and vaporization. Since n-heptane is also included as a component in the gasoline surrogate (as described below), the reaction mechanism for the diesel fuel is a subset of the gasoline surrogate reaction mechanism.

GASOLINE SURROGATE

Three surrogate fuel working groups published recommendations in 2007 for assembling surrogates for gasoline [4], diesel [5] and jet fuels [6]. Subsequent work has been performed by Naik et al. [7] to further explore appropriate surrogate components for gasoline and diesel, as part of work supported by the Model Fuels Consortium [8]. This effort has included assembling a database of component-fuel mechanisms to support representation of a wider range of

fuel properties. The choice of the components in this work draws from these studies. Each surrogate component represents a chemical class, as shown in [Table 1](#).

A software program called the Surrogate Blend Optimizer that is part of the Reaction Workbench [9] was used for determining the optimum surrogate. Appropriate model-fuel components are selected from a palette of options. Then, based on selection of several fuel-property targets, we determine the optimum model-fuel blend. The targets specified include the fuel RON and MON (autoignition resistance), the H/C ratio (sooting tendency), the lower heating value (LHV, i.e., the heat content), the liquid density and the T50 (temperature at which 50 mass % evaporates). The surrogate RON and MON calculations accounted for non-linear dependencies of fuel composition, based on the correlations of Ghosh et al. [10].

Using this method, we identified a 5-component gasoline surrogate shown in [Table 1](#), matching properties of the specific gasoline used in the engine experiments, n-alkanes, iso-alkanes, aromatics and alkenes are represented by the surrogate components. Since iso-alkanes are a major constituent of gasoline, two surrogate components from this class (iso-octane and iso-hexane) covering a range of fuel properties have been included for the gasoline surrogate. Relative to other chemical classes, typically cycloalkanes make up only a small portion of gasoline, and hence have not been considered in the gasoline surrogate.

[Table 2](#) shows that the surrogate is able to reproduce most of the measured gasoline properties well. Since some properties were not available for the gasoline used in the engine experiments, [Table 2](#) compares other properties with a typical range of gasoline properties reported by Pitz et al. [4] and Naik et al. [7]. Gasoline composition varies in different regions such as the US, Japan and Europe. The approach used in this work allows tailoring of the model fuel to the specifications of the market fuel of interest. In this way it may also be used to explore the effects of fuel variability on the engine performance.

THE CASE FOR A COMPLEX SURROGATE

In this study, we sought to understand and quantify the differences that result from using the multi-component gasoline surrogate shown in [Table 1](#), compared to the one-component surrogate of Kokjohn et al. [1]. This would help determine when the accuracy improvement justifies the extra computational cost of the complex surrogate.

Under HCCI engine conditions, it has been observed that RON or MON alone are not good indicators of ignition quality. Under these conditions, fuel reactivity has been reported to be better correlated experimentally with the

Table 1. Composition of the gasoline surrogate

Model Fuel Components	Representing chemical class	Liquid volume %
Toluene	Aromatics	35
1-Hexene	Alkene	13
iso-Hexane	iso-Alkane	10
iso-Octane	iso-Alkane	33
n-Heptane	n-Alkane	9

gasoline fuel sensitivity (i.e., RON-MON) [11, 12]. Kalghatgi et al. [11] suggested that fuel sensitivity and RON are most relevant to fuel reactivity under HCCI conditions, while Bunting et al. [12] suggested that fuel sensitivity and MON are most relevant to representing HCCI conditions [12]. Engine experiments of Bunting et al. [12] conducted under HCCI conditions showed that a PRF surrogate (n-heptane/iso-octane) with the correct octane number $[(RON+MON)/2]$ could not adequately capture gasoline ignition timing. This could be explained by the fact that a gasoline PRF has zero fuel sensitivity by definition (RON and MON have the same value for both n-heptane and iso-octane), while market gasoline typically has a sensitivity of ~ 12 .

An accurate surrogate should be able to predict the different behavior of the fuel under the RON and MON engine conditions. HCCI engine conditions vary over a wide range, and are quite different from either the RON or MON test conditions. While matching the gasoline sensitivity by itself does not guarantee that the surrogate can accurately predict gasoline reactivity under various HCCI engine conditions, in combination with matching other gasoline fuel properties, the surrogate has a better chance of modeling gasoline HCCI reactivity.

The surrogate generated in this work (Table 1) represents the fuel sensitivity, RON and MON well. Single-component surrogates, and the simple PRF have zero fuel sensitivity. Toluene reference fuels (TRF = toluene/n-heptane/iso-octane blends) have some fuel sensitivity, but the sensitivity would be due to toluene alone. Using a TRF to represent gasoline fuels with high fuel sensitivity would lead to surrogates with unrealistically large quantities of toluene. For accurately representing fuel sensitivity, then, it is better to have several surrogate-fuel components, as used in this work.

To quantify the difference in results between using the surrogate in Table 1 and the iso-octane-only gasoline surrogate, we performed some simulations for engine

conditions of the dual-fuel engine for a nominal load of 11 bar IMEP (127 mg/cycle total fuel). The fuel reactivity (gasoline vs. diesel content) and EGR rate were varied, and the impact on ignition timing (as defined by CA50) was studied. All other model inputs were maintained at the same values for all cases. In the simulation results presented below, the diesel surrogate used for both cases is the one-component n-heptane model described earlier.

For simplicity, the CHEMKIN-PRO zero-dimensional single-zone internal combustion engine model [13], under adiabatic conditions, was used for this comparison. While the zero-dimensional model is not appropriate for modeling the combustion duration and emissions, it can predict the trends for ignition timing reasonably well. The same kinetics mechanism was used for both surrogates, which was an un-reduced master mechanism consisting of 2099 species and 9789 reactions that is described in the next section.

Figure 1 shows the calculated effects of EGR rate and gasoline mass on combustion phasing at a fixed total fuel mass of 127 mg/cycle (nominal load of 11 bar IMEP). The simulations started at -95° ATDC, and the starting temperature and pressure were 387 K and 3.3 bar respectively. The compression ratio was 16.1:1 and the displacement volume was 2440 cm³. Note that, in the simulations in Figure 1, EGR was assumed to consist of only the saturated products of complete combustion (i.e., CO₂, H₂O, N₂, and O₂). The mixture becomes less reactive when gasoline-to-diesel ratio in the dual-fuel operation is increased (less reactive fuel), and as the EGR rate is increased (more dilution). As the mixture becomes less reactive due to these two factors, the single-component gasoline surrogate shows much earlier misfire, due to lower reactivity. The more reactive components of the multi-component surrogate, which contribute to fuel sensitivity, enhance fuel reactivity at these conditions, such that misfire is avoided.

Table 2. Comparison of surrogate properties with gasoline properties (properties of gasoline used in engine tests are highlighted in bold; other properties are ranges available in the literature [4, 7]).

	Gasoline	5-component surrogate
RON	95.6	95.9
MON	87.8	86.7
Sensitivity (=RON-MON)	7.8	9.2
Lower heating value (MJ/kg)	43.2	43.1
Molar H/C ratio	1.88	1.76
Liquid density (kg/m³)	756	743
Temperature 50 mass % evaporated (K)	378	372
Aromatics content (vol %) [4]	10-45	35
n- and iso-alkanes content (vol %) [4]	33-79	52
Alkenes content (vol %) [4]	1-18	13
Naphthenes content (liquid vol %) [4]	2-10	0
Average molecular weight (g/mol) [7]	98.9-105	96.7
Average formula [7]	C _{7.3} H _{14.8}	C ₇ H _{12.4}
Carbon number range [7]	4-12 (5-8 dominates)	6-8

It may be noted that the use of a small amount of diesel in dual-fuel engines plays a large role in promoting initial reactivity, and this reduces the need for a complex surrogate. However, to accurately model several mixtures of gasoline and diesel, using complex surrogates is recommended.

Quantifying the temperature needed for ignition to occur at a specific point (e.g., TDC) as the fuel reactivity changes (gasoline vs. diesel content) is another way to understand the differences between the multi-component and single-component surrogates. This is shown in [Figure 2](#). The starting pressure (3.3 bar) and equivalence ratios (0.77) are the same for all the cases; the mass changes due to changes in temperature. The simulations started at -95° ATDC. The compression ratio was 16.1:1 and the displacement volume was 2440 cm³. The CHEMKIN-PRO zero-dimensional single-zone model [13] was again used under adiabatic conditions, with the same master reaction mechanism for all cases, as in [Figure 1](#).

In addition to the 5-component and 1-component gasoline surrogates, the results using a PRF 91 surrogate (n-heptane/iso-octane) has also been included in [Figure 2](#). For less reactive fuels (more gasoline content), the 1-component surrogate shows significantly lower reactivity than the multi-component surrogate. Kokjohn et al. determined that around 80% gasoline/20% diesel has optimal fuel reactivity [1]. At those conditions, the 1-component surrogate simulations suggests that 60 K higher starting temperature is needed, compared to the multi-component surrogate simulations, to achieve ignition at TDC. The PRF surrogate reactivity lies in between the 1-component and 5-component gasoline surrogates. It may be noted that the analyses shown in [Figure 1](#) and [Figure 2](#) are based only on simulations, and no corresponding experimental data are available for comparison.

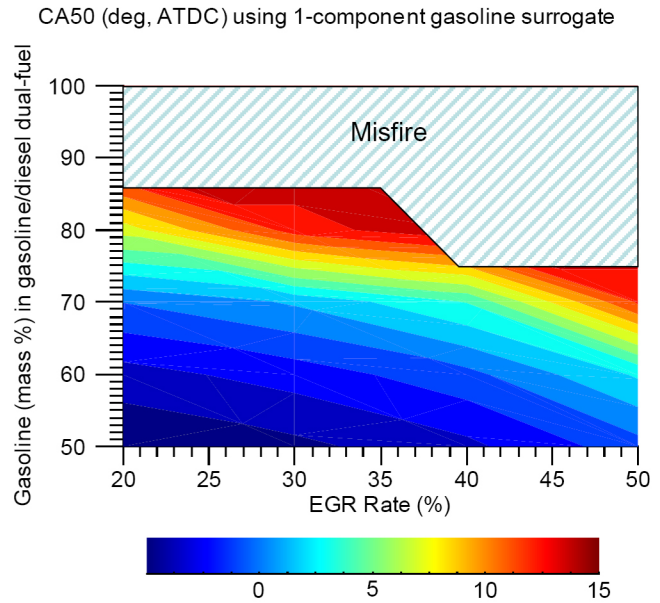
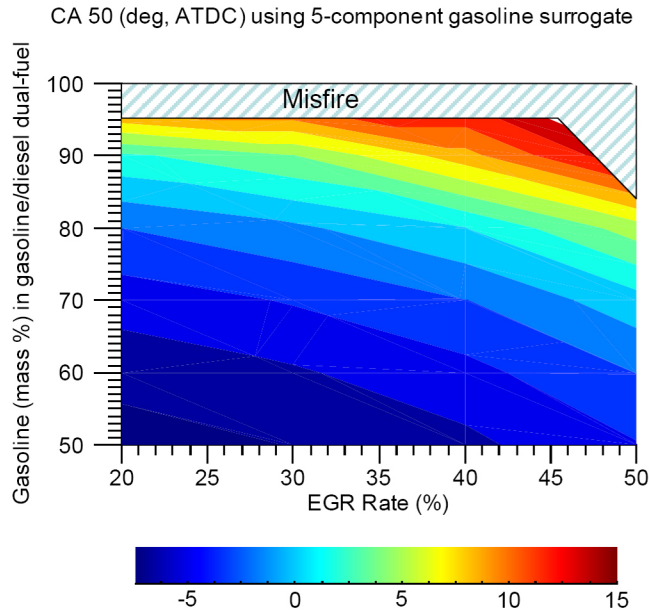


Figure 1. Comparison of ignition predictions using a single-component (iso-octane) gasoline surrogate to that using the detailed gasoline surrogate shown in Table 1. The simulation used a single-zone HCCI engine model, varying EGR rate and fuel reactivity, for a dual-fuel case with a nominal load of 11 bar IMEP.

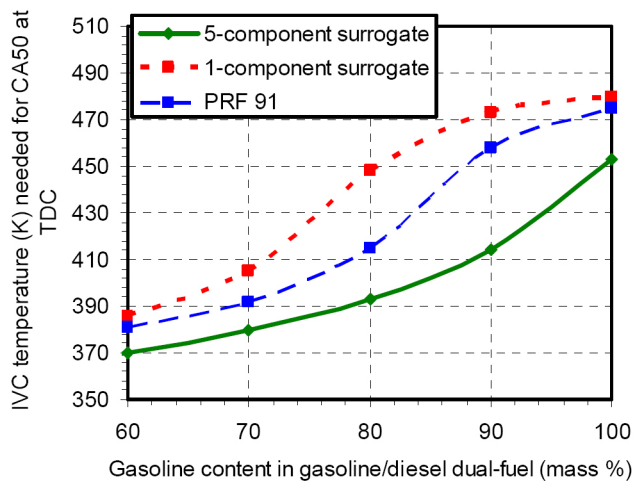


Figure 2. Quantifying the temperature needed for ignition to occur at TDC as the fuel reactivity changes (gasoline vs. diesel content), for simulations using single-component vs. multi-component surrogates. A zero-dimensional single-zone HCCI engine model was used. 40% EGR conditions are used for a dual-fuel case with a nominal load of 11 bar IMEP.

REACTION MECHANISMS FOR 3-D CFD SIMULATIONS

In other work, we have assembled a detailed master kinetic mechanism that includes a palette of validated surrogate-fuel components that have been tested over a wide range of conditions [8, 14, 15, 16]. From this detailed mechanism, we

have extracted reduced mechanisms for the specific surrogate fuel blend described above and for the operating conditions of the dual-fuel engine experiments. The detailed master mechanism used in this work consists of 2099 species and 9789 reactions, and has been developed as part of the Model Fuels Consortium [8]. The mechanism can model the combustion chemistry of twenty-eight surrogate fuels, and uses self-consistent core sub-mechanisms. Some of the relevant mechanism validation results are presented below to establish the fundamental nature of the mechanism. This is followed by a description of the mechanism reduction process and the resulting reduced mechanisms used in the CFD simulations.

VALIDATION OF THE MASTER MECHANISM

Before using reaction mechanisms in complex engine simulations, it is important to assess the validity of the mechanism over a wide range of conditions, as determined by comparison to fundamental experiments that can be modeled in a straightforward way. Here we present results from such tests of our master mechanism, for the most relevant cases of a more-extensive mechanism validation project. Table 3 lists the cases reported for pure components, and Table 4 lists the cases for the gasoline, diesel and fuel blends. The range of conditions covered include pyrolysis and oxidation conditions, pressures of 1-50 atm, and temperatures of 650-1800 K, as listed in Table 3 and Table 4. The tables list the sources for the experimental data. The data considered are from well defined laboratory experiments, which include

Table 3. Summary of validation data for pure surrogate components

Fig. #	Fuel	Source	Experiment type	Temp (K)	Pressure (atm)	Equivalence ratio	Dilution
(a)	n-heptane	Shen et al. [20]	Shock tube	780-1230	50	0.2-1	Oxidation in air
(b)	n-heptane	Ciezki et al. [21]	Shock tube	650-1350	40	0.5-2	Oxidation in air
(c)	n-heptane	Garner et al. [22]	Shock tube (species profiles)	900-1300	50	pyrolysis	99.99 mol% Ar
(d), (e)	iso-octane	Davidson et al. [23]	Shock tube	1100-1800	1.5	0.5-2	93-99 mol% Ar dilution
(f)	toluene	Vasudevan et al. [24]	Shock tube	1400-1850	2-3	0.5-1.5	95-99 mol% Ar dilution
(g)	toluene	Shen et al. [25]	Shock tube	1050-1250	50	0.25-1	Oxidation in air
(h), (i)	toluene	Klotz et al. [18]	Flow reactor	1173	1	0.76	~98 mol% N ₂ dilution
(j)	toluene	Dagaut et al. [26]	Jet-stirred reactor	1000-1400	1	1	98.5 mol% N ₂ dilution
(k)	1-hexene	Yahyaoui et al. [27]	Shock tube	1300-1800	10	1	99 mol% Ar dilution
(l)	1-hexene	Vanhove et al. [28]	RCM	650-850	6.2-8.5	1	79 mol % Ar/N ₂ /CO ₂

ignition times from shock tubes and rapid compression machines (RCM), species profiles from jet-stirred reactors and flow reactors. Other validation tests performed that are not reported here due to their lower direct relevance include comparisons of laminar flame speeds, extinction strain rates, and species profiles from burner-stabilized flames and opposed-flow flames.

CHEMKIN-PRO [13] reactor models were used for the mechanism validation modeling. The reflected shock experiments were modeled using the a closed homogeneous reactor model under constant volume conditions; the rapid-compression machine (RCM) experiments were modeled from the end of compression using the closed homogeneous reactor model under constant volume conditions; the jet-stirred reactor experiments were modeled using a perfectly stirred reactor model under steady-state conditions; flow reactor experiments were modeled using the closed homogeneous reactor model under isobaric conditions, an approach similar to that of others [17, 18, 19].

All the calculated ignition times are based on temperature inflection; for most of the conditions, ignition times calculated using other definitions, such as peak OH, resulted

in very similar values. All these mechanism-validation simulations were performed under adiabatic conditions. The only experiments that involve significant heat losses are those from the RCM. For the RCM conditions, the ignition times considered extend up to 0.1 sec, which could result in heat loss effects; however, since heat losses are not well defined, simulations have been performed under adiabatic conditions, such that the predictions are expected to give smaller ignition times than those measured.

Figure 3 shows the comparisons of model predictions and experimental data for pure components, and Figure 4 shows the comparisons for blends and real fuels. Most of the validation cases show good agreement between the model predictions and the experimental data over the wide range of conditions considered. Matching species profiles in addition to ignition times provides more confidence in the reaction pathways. Some cases, such as 1-hexene ignition times under low-temperature conditions, show some discrepancies. However, overall, the component models and component blends show good agreement with the wide range of data considered.

Table 4. Summary of validation data for surrogate fuel blends

Fig. #	Fuel	Source	Experiment type	Temp (K)	Pressure (atm)	Equivalence ratio	Dilution
(m)	Gasoline (modeled using 5-component surrogate)	Gauthier et al. [23]	Shock tube	900-1100	50	0.5-1	Oxidizer is air
(n)	Diesel (modeled using 1-component surrogate)	Haylett et al. [29]	Shock tube	900-1300	6	0.5	79 mol% Ar
(o)	PRF100, PRF80, PRF60, PRF0	Fieweger et al. [30]	Shock tube	700-1100	40	1	Oxidizer is air
(p)	PRF0, PRF80, PRF100	Griffiths et al. [31]	RCM	650-1000	131 mol/m ³ compressed charge density	1	79 mol % Ar/N ₂ /CO ₂
(q)	PRF90	Callahan et al. [32]	RCM	650-900	266 mol/m ³ compressed charge density	1	79 mol % Ar/N ₂ /CO ₂
(r), (s)	PRF87	Callahan et al. [32]	Flow reactor	550-850	12.5	1	98 mol % N ₂
(t)	n-heptane (17 mol%) +iso-octane (63%) +toluene (20%)	Gauthier et al. [23]	Shock tube	1000-1150	25-50	1	Oxidizer is air
(u)	iso-octane (45 mol%) +1-hexene (13.5%) +toluene(31.5%) +ETBE(10%)	Yahyaoui et al. [27]	Jet-stirred reactor	750-1100	10	1	98.84 mol% N ₂
(v)	iso-octane (45 mol%) +1-hexene (13.5%) +toluene(31.5%) +ETBE(10%)	Yahyaoui et al. [27]	Shock tube	1300-1800	10	1	0.1 mol% fuel, diluted in Ar
(w)	iso-octane (20.9 mol%) +n-heptane (6.3%)+toluene(10.2%) +ethanol(62.4%)	Cancino et al. [33]	Shock tube	700-1200	10-30	1	Oxidizer is air
(x)	PRF[0-100]/air	Tanaka et al. [34]	RCM	~840 K	613 mol/m ³ compressed charge density	0.4	Oxidizer is air

TARGETED MECHANISM REDUCTION

The reaction pathways needed for the surrogate used in this work are a small subset of the 28-component master mechanism. Hence, for the HCCI and RCCI engine conditions, targeted mechanism reduction was performed prior to the CFD calculations. The HCCI and RCCI engine

operating conditions differed, with the RCCI engine involving more fuel stratification and a higher EGR. In the interests of using the smallest possible reduced mechanisms for CFD calculations, two different reduced mechanisms were generated for targeted HCCI and RCCI engine conditions. The reduced mechanism is skeletal in the sense that it was created by removing species and associated



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