A parametric investigation of HCCI operating conditions on engine performance characteristics using detailed kinetic simulations

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Abstract
The work investigates the effect of key operating parameters on performance and pollutant characteristics of a Homogeneous Charge Compression Ignition engine. An accredited detailed chemical kinetic mechanism for gasoline surrogate components, coupled with a NO_x sub-mechanism, is implemented on a commercial 0-D single zone, engine model. The simulations target on identifying optimum performance guidelines regarding operating parameters using typical primary reference fuels on the geometry of a widely investigated research engine. The effect of primary reference fuels, intake charge and EGR levels is discussed based on pressure traces, heat release rate profiles and combustion phasing analyses. The work also explores the applicability and limitations of such an approach and investigates the extent to which a solid methodological approach based on detailed kinetic models, could be helpful for gaining some chemical insight on the heat release and pollutant formation processes.

Acronyms

ICE	Internal Combustion Engine
LTC	Low Temperature Combustion
SI	Spark ignition
CI	Compression ignition
HCCI	Homogenous-Charge Compression-Ignition
SCCI	Stratified-Charge Compression-Ignition
PCCI	Premixed Charge Compression Ignition
RCCI	Reactivity Controlled Compression Ignition
PFS-CI	Partial Fuel Stratification
EGR	Exhaust Gas Recirculation
RON	Research Octane Number
MON	Motor Octane Number
CN	Cetane Number
IVC	Inlet valve opening
EVO	Exhaust valve opening
TDC	Top dead center
IMEP	Indicative Mean Effective Pressure
CA*x*	Crank Angle for *x* % heat release
HRR	Heat Release, Heat Release Rate
PPRR	Peak Pressure Rise Rate

Introduction

The current overspending of primary energy resources and increased environmental concerns, call for optimization of the engine conversion process, also through the introduction of new technological concepts and novel fuels. Based on almost all relevant projections and technology assessment reviews [1, 2], the internal combustion engine (ICE) will retain its leading role in land and sea transport, particularly for intermediate and long distances, in the near future.

The quest for thermal engines that can substantially improve thermal efficiency and reduce exhaust emissions in order to simultaneously address stringent emission limitations, has led to the investigation of novel combustion modes. Modern trends in engine design include complex fuel injection control strategies and/or Exhaust Gas Recirculation (EGR). Efforts to move away from conventional flames (collectively characterized by high temperatures, significant heat losses, sooty behavior) and go towards regimes characterized by high mixing, low temperatures and controlled heat release rates, have been conducted. The strategies following the aforementioned principles can be generally characterized as Low Temperature Combustion (LTC) modes. LTC can be beneficial both for NO_x reduction, due to the lower system temperatures, and soot reduction, due to better mixing conditions, as well [3].

Efforts to achieve practical engine operation under the LTC concept, have led to the development of new combustion strategies, such as Homogenous-Charge Compression-Ignition (HCCI), Stratified-Charge Compression-Ignition (SCCI), Premixed Charge Compression Ignition (PCCI), Reactivity Controlled Compression Ignition (RCCI), Partial Fuel Stratification Compression Ignition (PFS-CI) [3-5]. In each of the aforementioned combustion modes, charge homogeneity and combustion timing are the two key parameters controlling the combustion process.

HCCI injects fuel during the intake stroke and a premixed mixture of fuel and air (homogeneous charge) are compressed to the point of auto-ignition (spontaneously for the entire mixture). However, since ignition timing is not explicitly governed by a spark plug (like in SI engines) or fuel injection (as in diesel CI engines), the reactivity of the charge largely controls the combustion event. Following the underlying principle of the LTC concept, HCCI has been shown to be thermally efficient and results in lower NO_x and particulate matter (PM), but relatively high emissions of hydrocarbons (HC) and CO [6].

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Like HCCI, SCCI also increases temperature and density during the compression stroke, however, the fuel is injected later. Combustion occurs at the boundary of the fuel and air, producing higher emissions, but under overall leaner charge and results in higher efficiency [7]. PCCI combustion is a hybrid mode between HCCI and CI combustion; the fuel is injected early during compression stroke to promote mixing prior to ignition in such a way that the coupling between the start of fuel injection and the start of combustion is maintained [8]. RCCI is a dual fuel engine combustion technology featuring enhanced controllability of combustion. It has the potential for lower fuel consumption and emissions via in-cylinder fuel blending (two or more fuels) of different reactivity and multiple injections so as to control charge reactivity and to optimize combustion phasing and duration [9]. A review on the LTC strategies for advanced CI engines can be found in [10].

The control of ignition timing and heat release rate is the most crucial factor in *xCCI* ($x = H, S, P, R$) modes, particularly under high and full load operation. Charge auto-ignition is governed by chemical kinetics, thus control over combustion phasing requires tuning of the auto-ignition kinetics, which is in turn affected by the mixture equivalence ratio and the thermodynamic state of the reactants during the compression process. The ignition delay is controlled by the formation of intermediate species which subsequently react during the low-temperature oxidation regime of hydrocarbon fuels [11].

EGR strategies have been proposed as an effective means of controlling combustion and reducing NO_x emissions. The application of EGR in IC engines involves replacement of some of the inlet air with the exhaust from a previous cycle, or direct addition of the exhaust gases to the inlet air stream. As a result, the inlet charge is diluted and its heat capacity is increased, which in turn lower the combustion temperature and NO_x emissions. LTC strategies implement EGR in combination with different fuel injection strategies, in order to achieve the desired Heat Release Rate (HRR) profile and emissions characteristics, offering up to 20% improved fuel efficiency in comparison to conventional diesel, and 40–50% in comparison to conventional SI gasoline engine, e.g. [3]. However, LTC regimes function under conditions which are near to typical engine operational limits [11].

Currently, the fuels used in IC engines are gasoline, for SI ICE (light duty applications), and diesel, for CI ICE (mostly medium and heavy duty applications). Both fuels are complex blends of hydrocarbons. The primary fuel property is the auto-ignition quality: gasolines are resistant to auto-ignition to avoid knock (measured by octane numbers, RON and MON) while diesel fuels are prone to auto-ignition (measured by Cetane Number, CN) [12].

While the desired fuel properties can be considered well defined for the cases of typical SI and CI engines, for the HCCI case the ideal fuel property palette is not that obvious. Recently, it has been suggested, that a possible efficient coupling between advanced (fossil-based) transportation fuels and modern engines, would involve the use of gasoline-like fuels in CI-like engines [12].

From all the above, it is clear that an holistic approach taking into account the interplay of *fuel properties* (RON, MON, CN or other auto-ignition related indices), *combustion mode* (SI, CI, xCCI) and *operating conditions* (charge stoichiometry, intake thermodynamic conditions, engine speed), for a particular *engine design* (displacement volume, compression ratio, valve timings), should be followed so as to further facilitate the effect of each parameter in a concise and straightforward way. The concurrent assessment of engine efficiency and pollutant formation, when a combination of advanced engines concepts and novel fuels is concerned, needs to be tackled through a detailed kinetics approach able to provide insight on the respective chemistry issues, *e.g.* [13], and, ideally, using a realistic turbulent full 3-D CFD simulation framework.

Scope of this work is to perform a parametric investigation of HCCI operating conditions on engine performance characteristics using detailed kinetic simulations in a homogeneous 0-D environment. A series of chemical kinetic simulations for realistic operation conditions of a commonly used single-cylinder research Hydra engine (see Table 1) have been performed on the basis of published and appropriately validated kinetic schemes.

The structure of the paper is as follows: first the numerical approach followed herein is presented. Then, the framework of the parametric investigation, namely the engine geometric and operation characteristics, are described for each of the cases investigated. Having set the basis of the work, simulation results including in-cylinder pressure, temperature and heat release histories, as well as specific kinetic information, are discussed. Particular attention is paid on the effect of EGR. Finally, the paper concludes summarizing the main findings of the parametric investigation and underlying future relevant work.

Numerical approach

In the present work, the 0-D single zone engine model of the CHEMKIN 4.1 suite has been used [14]. The code solves the transient form of the conservation equations of mass, energy, and species for a perfectly mixed (thus, “homogeneous”) reactor. Practically, it accounts for temperature, pressure and species evolution from IVC to EVO (i.e. closed system).

The applicability of 0-D single zone approaches for HCCI investigations has been demonstrated in the literature in various studies, e.g. [15-19], all taking advance of CHEMKIN’s capability of easy and efficient (short computational times) handling of large detailed chemical kinetic schemes, thus making it a useful tool when the effects of fuel surrogate chemistry on the ignition timing are concerned.

The LLNL gasoline surrogate detailed kinetic mechanism of [20] has been augmented with the NO_x chemistry of the GRI 3.0 mechanism [21] and has been utilized thought this exercise. The resulting mechanism comprises of 6041 reactions among 1406 species, including linear and branched saturated hydrocarbons, olefins, and aromatics. The mechanism has been shown to very accurately reproduce the ignition delay times of single gasoline components and their binary and multi-component mixtures in rapid compression machines and shock tubes, as well as jet stirred reactors of a wide range of operating conditions pertinent to HCCI ICE operation [20].

The calibration of a heat transfer model for HCCI operation has been investigated in the literature, e.g. [22, 23] In the present work, heat transfer was modeled using the widely used following equation: $Nu = a*Re^b*Pr^c$ [14]. Based on previous related modelling studies of HCCI engines ([23], [24] as appears in [14]), the constants were chosen as $a = 0.035$, $b = 0.71$, $c = 0$. The cylinder wall temperature was set at 400 K. Additional, the coefficients for the Woschni equation [14, 25] for heat transfer were chosen from the literature as $c_{11} = 2.28$, $c_{12} = 0.308$, $c_2 = 3.24$ [20]. Brute force sensitivity computations on the heat transfer correlation parameters have not shown sensitivity on computational results. Note that single zone models, because of neglecting in-cylinder temperature and composition distribution, over-predict in-cylinder pressure. With the Woschni correlation, one still expects to achieve higher in-cylinder temperatures (due to lower heat flux). A methodology of a more suitable correlation for HCCI ICEs [22] is presented in [19] and will be implemented in a continuation of this work. The above study [19], also highlights the importance of the implemented heat transfer model when detailed kinetic simulations are compared against real experimental data.

Framework of the parametric investigation

The characteristics of the single cylinder Ricardo Hydra research engine, as appears in the work of [17, 18] and adopted in the present computational study, are presented in Table 1, together with the assumed operating conditions of the base case scenario.

Parameter	**Value**
Cylinders	1
Bore / Stroke	86/86 mm
Swept Volume	0.5 lt
IVC (deg aBDC)	44.0
EVO (deg bBDC)	42.0
Compression ratio	10.5:1
Speed	1200 rpm
Intake pressure	1.8 bar
Intake temperature	200^{o}C
Charge stoichiometry	0.2

Table 1. Engine characteristics and operating conditions of the base case configuration.

The parametric numerical investigation that has been conducted in the frame of the present work is as follows:

a) Base case configuration for 5 different fuels, as presented in Table 2.

b) For the base case configuration with the PRF80 fuel:

1. Global fuel-to-air stoichiometry ratio (φ): 0.2 and 0.4.
2. Intake air temperature: 150 – 200 – 250 ^{o}C
3. Boosting pressure: 1.8 – 2.5 bar abs.
4. EGR levels: 20 – 50 – 80%.

Fuel	**n-heptane**	**iso-octane**	**RON**	**LHV (kJ/mol)**
PRF0	100	0	0	4465.8
PRF40	60	40	40	4709.4
PRF60	40	60	60	4831.3
PRF80	20	80	80	4953.1
PRF100	0	100	100	5074.9

Table 2. Fuels considered in the parametric investigation.

The PRF80 fuel has been chosen in order to be in line with the findings of [12]. Under the examined operating conditions, the fuels considered and the choice of the charge stoichiometry, computed IMEP range from ca. 3.5 to 7.8 bar. EGR has been simulated as a pure CO_2 stream and is defined as: $EGR(\%)=X_{CO_2\_intake}/X_{CO_2\_exhaust}$ [26].

Fuel effects (RON sensitivity)

Pressure history and heat-release distribution in practical engines is crucial, not only for the identification of energy intensive regions but also for the understanding and prediction of combustion instabilities and combustion noise, e.g. [27]. Figure 1 presents the in-cylinder pressure and HR evolution and for five different PRF fuels. Moving towards less reactive fuels (higher RON), two stage mixture ignition is diminished, combustion duration (as indicated by the difference CA90-CA10) decreases and peak pressure rise rate (PPRR) is increased. It is interesting to note that the cumulative heat release remains practically constant and IMEP varies within less than 15%.

Intake charge conditions (T, p, ϕ sensitivity)

The effect of intake temperature on the pressure and HRR is shown in Fig. 2 for the case of a PFF80 fuel. The $T_{in} = 150$ ^{o}C does not result in an ignition event, at least for the specific geometric and operation characteristics of the present study. Higher intake temperature results in earlier combustion timing and higher PPRR.

Higher intake pressure also promotes combustion, increases charge reactivity and result in earlier combustion timing and short combustion duration (see Fig. 3 and Table 2). With higher boosting at the manifold at 2.5 bar, the peak in-cylinder pressure climbs to 84 atm just before the TDC (from a value of 59 atm in the 1.8 bar intake pressure). Naturally, the IMEP of the higher pressure case is about 35% higher than the lower one.

Case	CA50 (deg)	Combustion duration (deg)	PPRR (bar/deg)
PRF0	-20.0	17.0	1.30
PRF40	-15.2	6.8	4.57
PRF60	-10.2	4.6	5.95
PRF80	0.52	3.7	7.64
PRF100	2.25	4.1	7.45
PRF80 T_{in}=250°C	-10.6	2.3	8.83
PRF80 p_{in}=2.5 bar	-5.1	3.1	13.44
PRF80 ϕ = 0.4	-2.3	0.8	384.2
PRF40 ϕ = 0.4	-24.1	2.1	168.2

Table 3. Global combustion characteristics for the cases presented in Figure 1.

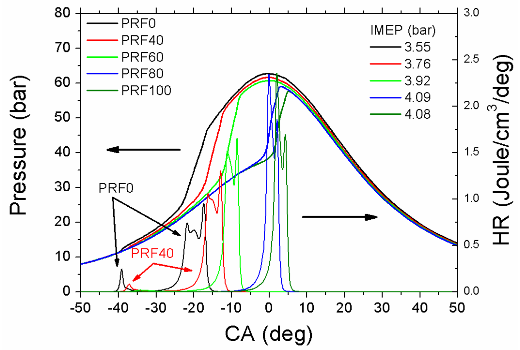

Figure 1. Pressure and HRR traces for five fuels of different RON values.

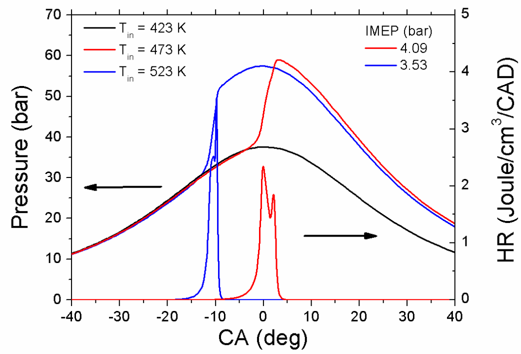

Figure 2. Intake temperature effect on pressure and HRR for a PRF with RON80.

Charge stoichiometry (as expressed with the equivalent ratio ϕ) is directly linked to engine load and therefore it is important to study the ϕ-sensitivity of a particular fuel for a given set of engine characteristics [11]. The effect of the charge stoichiometry for the PRF80 fuel is presented in Fig. 4 below. The richer mixture features double cumulative HR and, naturally, 45% more heat losses. Richer charge operation results in a very steep HRR and consequently, to a large PPRR, confirming the limitation of the HCCI concept on high load operation. Although PFS has been proposed as an effective means of tackling this issue, it has also been found that suitable fuels for medium load HCCI operation (i.e. RON 65-85 [12]) may not be the most appropriate for PFS application; fuels of lower RON exhibiting a stronger two-stage ignition behavior would benefit a PFS HCCI operation. Indeed, computations with a PRF40 fuel has shown a 55% reduction of the PPRR (conditions as those of Fig. 4 with ϕ = 0.4, IMEP = 6.71 atm).

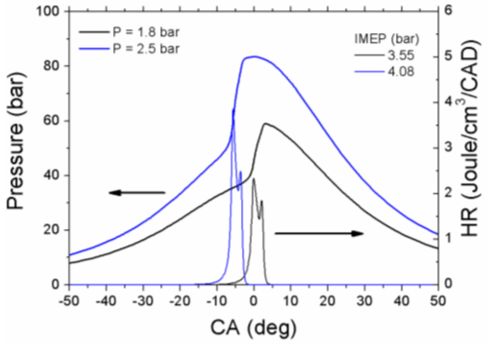

Figure 3. Effect of boosting pressure on pressure and HR for a PRF with RON80.

Combustion phasing will be also affected at higher load, see Table 2. For the lower RON case, the two-stage ignition behavior further reduced the CA degrees of CA50 while combustion duration is increased.

Stoichiometry sensitivity at increased pressure conditions will be analyzed in a future work; however, it is anticipated that for gasoline-like fuels (high RON), increased pressures will result in high f-sensitive operation, primarily due to the effect of pressure on the reactions controlling the intermediate temperature heat release (ITHR) [11, 19, 20].

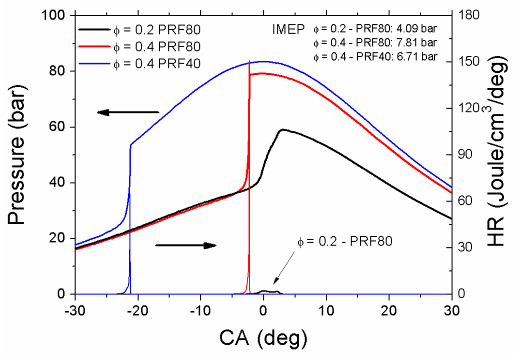

Figure 4. Stoichiometry charge sensitivity of pressure and HRR traces for two fuels.

EGR investigation

In conventional (mainly CI) ICE engines, EGR is primarily implemented for controlling NO_x via the in-cylinder temperature reduction. In HCCI engines, EGR can be used also as a means of controlling the pressure rise rate, particularly at higher loads. Here, three different EGR rates are numerically examined for the base case engine configuration and a PRF80 fuel.

EGR (%)	Peak T (K)	Peak P (bar)	PPRR (bar/deg)	CA50 (deg)	CA90-CA10 (deg)
0	1642	59.8	7.65	0.52	3.7
20	1631	59.1	7.22	1.07	4.0
50	1613	57.8	6.63	2.01	4.17
80	1592	56.0	6.01	2.99	4.81

Table 3. In-cylinder peak temperature, peak pressure and CA50 at varying EGR levels.

In-cylinder temperature evolution is shown in Fig. 5, where up to a 3% reduction in the peak temperature and a 6% in the peak pressure is observed (see Table 3). Furthermore, the main phase of the combustion event moves later in time as this is indicated by a relevant shift of CA50 from ca. 0.5 deg (0% EGR) to ca. 3 deg (80% EGR). It is anticipated, that the effect of EGR would be more prominent on the case of engine operation with a fuel of lower RON; additional investigation will be presented in the poster version of this work. Note that computations also confirm a drop in the peak value of the pressure rise rate as EGR levels increase.

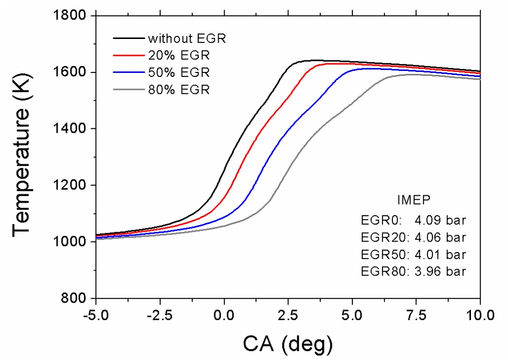

Figure 5. Effect of EGR levels on the in-cylinder temperature levels.

The differences in the thermodynamic conditions due to varying EGR levels (see Table 3), largely affects the total NO_x formation rate and exhaust levels (see Fig. 6). Peak total NO_x production rate is reduced by almost 55% resulting in a more than 40% reduction in the respective exhaust values. Note the compatibility of each total NO_x production rate profile shape with the respective combustion phasing and duration (Fig. 6 and Table 3), indicating the importance of the PHH pattern for NO_x control.

In-cylinder kinetics

A merit of the present detailed kinetics approach is the opportunity of gaining a chemical insight on the in-cylinder composition. Focusing on the base case simulation of this work, 11 species are found to have higher mole fraction values than 1 ppm in the peak pressure CA and 73 species in peak HRR CA position. Besides the typical species (fuel, N_2, O_2, CO, CO_2, H_2O, CH_4, C_2H_4), it is also interesting to note the evolution of key oxygenated species of different classes like acrolein (C_2H_3CHO – aldehyde) and iso-propanol i-C_3H_5OH (alcohol), see Fig. 7, cf. Fig. 2. Such findings are expected to be very case dependent; fuel composition and HRR pattern (one or two stage-ignition) would largely determine the fate of the intermediate species. Although in this particular case the above species are primarily consumed within the engine cycle, they could potentially survive at the exhaust providing that operating conditions are promoting their formation.

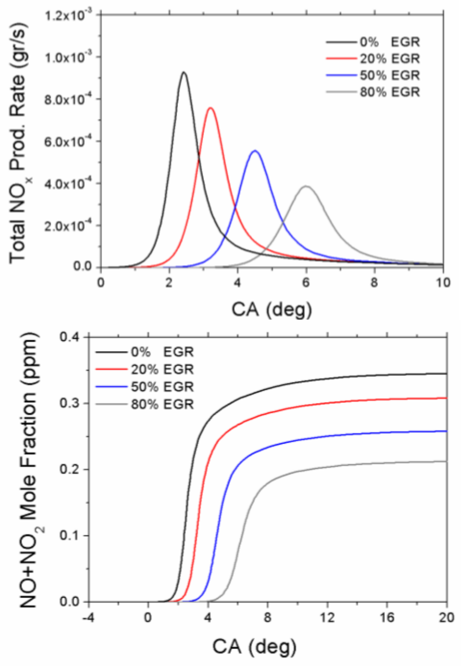

Figure 6. Effect of EGR levels on total NO_x production rate and NO and NO_2 levels.

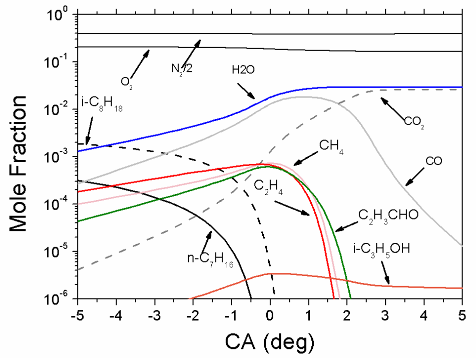

Figure 7. Effect of EGR levels on total NO_x production rate and NO and NO_2 levels.

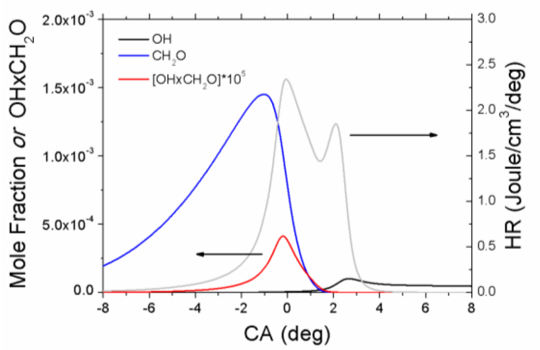

Figure 8. Effect of EGR levels on total NO_x production rate and NO and NO_2 levels.

Based on such chemical resolution, one can also investigate the appropriateness of proposed HRR correlations [28]. Figure 6 presents the OH, CH_2O, OH*x*CH_2O and HRR profiles. It is shown that the specific predicted HRR pattern cannot be capture with such a marker. However, this cannot be generalized. Further investigation on the validity of such a correlation should involve deep analysis of the detailed kinetic mechanism to reveal causal relations between the proposed probes and fundamental flame chemistry.

Concluding remarks and further work

The work utilizes a detailed kinetic approach in order to investigate the effect of key operating parameters on performance and pollutant characteristics of HCCI engines. A parametric investigation on fuels, intake charge conditions, EGR levels has been performed. Simulation results, including in-cylinder pressure, temperature and heat release histories, as well as specific kinetic information, confirm the generic characteristics of the HCCI mode. Simulations of in-cylinder species profiles have shown the importance of different intermediates on each stage of the combustion process.

The effect of engine speed and the compression ratio will be investigated in the future, using, e.g., the geometry of [16], and also considering operation with EGR. Moreover, numerical work on the investigation of the effect of different surrogate fuel composition on the overall combustion process will be also carried out, highlighting the importance of the quest for a single, detailed enough, mechanism containing all appropriate surrogate components, allowing thus for a direct comparison of the effect of each component on the heat release and pollutant formation processes. A detailed analysis of HR regimes would further elucidate the controlling elementary steps.

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