

Principle of large component number in multicomponent fuel combustion – a Monte Carlo study

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Abstract

The current work expands on a recently proposed principle concerning the combustion chemistry of multicomponent real fuels. The principle of large (fuel) component number states that the high-temperature combustion chemistry behaviors of multicomponent real fuels become statistically and practically identical when the number of hydrocarbon components exceeds a critical value. Monte Carlo simulations are carried out here to sample fuel mixtures comprised from 2 to 18 compounds with hydrocarbon classes including *n*-alkane, *iso*-alkane, alkylated cyclohexane compounds and alkylated benzenes. It is found that the critical number of fuel components is between 12 and 14 above which typical global combustion properties, including ignition delay time, laminar flame speed, and extinction residence time in a perfectly stirred reactor, converge to their respective mean values with standard deviations smaller than any modern-day combustion experiments can discern, irrespective of the exact composition of the fuel mixture.

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1. Introduction

Real fuels are often complex mixtures of hydrocarbons. For example, a conventional Jet A fuel is comprised of several major classes of hydrocarbon compounds, including *n*-alkanes, *iso*-alkanes, cycloalkanes, and alkylbenzenes, each of which may contain over hundreds of species. Real fuels can also vary widely in class compositions. For example, major classes of compounds in jet fuels can vary by as much as a factor of two [1]. Fuel specifications and certifications, on the other hand,

use only a small set of fuel properties that are indirectly related to the composition at the best. In the case of jet fuels, they include the H/C ratio, lower heating value (LHV), and the mass content of the aromatics. The evidence that such a small number of properties are sufficient to specify the combustion properties of a jet fuel (and its safe use) suggests that the high-temperature combustion chemistry properties of a real fuel are not ultra-sensitive to its composition.

Indeed, Davidson et al. [2] concluded from a recent study that under comparable conditions, the high-temperature shock tube ignition delay times of a broad range of distillate fuels are statistically indistinguishable. In earlier work, we briefly explored the causes for this insensitivity [3] and

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found that over a narrow range of conditions, the ignition delay time and laminar flame speed are insensitive to fuel composition as long as the number of fuel components is large enough (>12 – 14). The insensitivity was attributed to the statistical effect that resembles the law of large numbers [4]. Hence, the principle of large component number was proposed and subsequently tested in studies of the pyrolysis and oxidation of jet and rocket fuels in shock tube, flow reactor and laminar premixed and non-premixed flames [3,5].

In the current work, we expanded our computational Monte Carlo and detailed kinetic modeling study to a wider range of high-temperature combustion problems. Random fuel mixtures with n ($n = 2, \dots, 18$) hydrocarbon compounds were sampled from a group of 18 neat compounds ranging in size from C_6 to C_{12} and hydrocarbon classes from n -alkane, iso -alkane (both lightly- and heavily-branched), alkylated cyclohexane compounds to alkylbenzenes. Ignition delay time, laminar flame speed, and extinction residence time in perfectly stirred reactor (PSR) were computed and their distributions were studied as a function of the number of components. The results support the principle of large component number over a wide range of thermodynamic conditions and combustion phenomena. The current finding also has implications in the surrogate fuel approach and formulations, as will be discussed in detail.

2. Simulation methods

Monte Carlo simulations were carried out using the JetSurF 2.0 [6] model, which describes the high-temperature combustion reactions of n -alkane and n -alkylcyclohexane. The chemistry of n -alkylbenzenes and iso -alkanes (neo -hexane and 2,2,4-trimethylpentane) was added into the JetSurF model from the reaction models of Lawrence Livermore National Laboratory and NUI Galway [7–9]. Finally, the reaction submodels of 2-methylpentane and 2,5-dimethylhexane were built in the present work using reaction class rules. The final reaction model, consisting of 445 species and 2771 reactions, are provided in the SPM.

Computations were performed using the Sandia ChemKin package [10]. Simulations of fuel pyrolysis were carried out in isobaric and adiabatic condition. The ignition delay time was defined as the time to the maximum derivative of pressure with respect to time under the constant volume and adiabatic assumption. The laminar flame speed was calculated using PREMIX [11] with multicomponent transport and thermal diffusion. The extinction residence time in adiabatic PSR was obtained by calculating the S -curve using the Sandia PSR code [12]. The extinction time is defined as the reaction time corresponding to the upper turning point of the S -curve.

3. Fuel components

Fuel components sampled in the Monte Carlo simulations are listed in Table 1. Four types and 18 hydrocarbon compounds in all are considered. The results from this and the past study [3] show that the 18-compound pool is sufficiently large since the combustion properties of a fuel mixture converges at ~ 12 fuel components. The hydrocarbon types considered are n -alkane, iso -alkane, n -alkylcyclohexane, and n -alkylbenzene, which are common in distillate fuels. Although dicycloparaffins, tricycloparaffins, and some cyclic aromatics (e.g. naphthalenes, indans, and tetralins) can also exist in real fuels, their contributions to the total fuel composition are usually too small to be of any importance insofar as the global combustion properties are concerned. These compounds may impact the sooting propensity of a fuel, but this is beyond the scope of the present study.

The pyrolysis chemistry of iso -alkane is dependent on its molecular structure perhaps more so than some other classes of the compounds. While a lightly branched iso -alkane behaves like n -alkane in that its pyrolysis produces mostly ethylene, a highly branched iso -alkane, e.g., 2,2,4-trimethylpentane, could produce iso -butene as the dominant pyrolysis product. Here, we considered four iso -alkane compounds, 2-methylpentane, neo -hexane and 2,5-dimethylhexane, and 2,2,4-trimethylpentane to represent the variation of possible iso -alkane structures. In the Monte Carlo simulation, we randomly drew n ($n = 2, \dots, 18$) components from Table 1 to create fuel mixtures. The fuel composition was also assigned randomly for each fuel mixtures. Examples of random samples can be found in the Supplementary Material.

4. Results and discussion

We first present selected sample results of laminar flame speed (S_u^0) calculations. About 100 Monte Carlo fuel mixture samples were generated for each of the 4-, 12- and 18-component fuel mixtures. The flame speeds were then computed in stoichiometric air at 1 atm pressure and 403 K unburned gas temperature. Figure 1 shows the distributions of the computed S_u^0 . The measured flame speeds of several jet fuels are also shown for comparison. For reference, the S_u^0 values for single-component fuels at the same condition vary from 51 to 62 cm/s (see, Table 1). With the 4-component fuel mixtures, the variation in the flame speed narrows quickly from those of the single-component fuel, giving a 2σ value of 2.8 cm/s. It is seen from Fig. 1 that by increasing the number of components in the fuel from 4 to 12, the distribution narrows further ($2\sigma = 1.5$ cm/s). With 18 fuel components, the 2σ value is reduced to 0.7 cm/s. The mean flame speed value changes little, from 57.6 cm/s at four

Table 1
List of fuel components considered and their properties.

No.	Component	Molecular formula	MW (kg/kmol)	H/C ratio	$h_{f,298K}^{\circ}$ (kcal/mol)	LHV (MJ/kg)	$S_u^{\circ a}$ (cm/s)
Normal alkanes							
1	<i>n</i> -heptane	<i>n</i> -C ₇ H ₁₆	100.2	2.29	-45.1	44.9	60.7
2	<i>n</i> -octane	<i>n</i> -C ₈ H ₁₈	114.2	2.25	-50.0	44.8	60.3
3	<i>n</i> -nonane	<i>n</i> -C ₉ H ₂₀	128.3	2.22	-54.9	44.7	60.0
4	<i>n</i> -decane	<i>n</i> -C ₁₀ H ₂₂	142.3	2.20	-59.8	44.6	60.0
5	<i>n</i> -dodecane	<i>n</i> -C ₁₂ H ₂₆	170.3	2.17	-69.7	44.5	59.9
Lightly branched <i>iso</i> -alkanes							
6	2-methylpentane	C ₅ H ₁₁ -2-CH ₃	86.2	2.33	-41.6	45.0	57.5
7	2,5-dimethylhexane	C ₆ H ₁₂ -2,5-CH ₃	114.2	2.25	-52.8	44.7	54.6
Highly branched <i>iso</i> -alkanes							
8	<i>neo</i> -hexane	<i>neo</i> -C ₆ H ₁₄	86.2	2.33	-45.2	44.8	55.5
9	2,2,4-trimethylpentane	<i>i</i> -C ₈ H ₁₈	114.2	2.25	-53.4	44.7	51.1
Normal alkylcyclohexanes							
10	cyclohexane	<i>c</i> -C ₆ H ₁₂	84.2	2.00	-29.5	43.8	61.7
11	methylcyclohexane	<i>c</i> -C ₆ H ₁₁ -CH ₃	98.2	2.00	-35.9	43.8	59.1
12	ethylcyclohexane	<i>c</i> -C ₆ H ₁₁ -C ₂ H ₅	112.2	2.00	-40.4	43.8	52.5
13	<i>n</i> -propylcyclohexane	<i>c</i> -C ₆ H ₁₁ - <i>n</i> -C ₃ H ₇	126.2	2.00	-45.4	43.8	57.3
14	<i>n</i> -butylcyclohexane	<i>c</i> -C ₆ H ₁₁ - <i>n</i> -C ₄ H ₉	140.3	2.00	-51.5	43.8	57.6
Normal alkylbenzenes							
15	toluene	C ₆ H ₅ CH ₃	92.1	1.14	12.0	40.9	52.9
16	ethylbenzene	C ₆ H ₅ C ₂ H ₅	106.2	1.25	7.0	41.3	58.5
17	<i>n</i> -propylbenzene	C ₆ H ₅ - <i>n</i> -C ₃ H ₇	120.2	1.33	1.9	41.6	56.4
18	<i>n</i> -butylbenzene	C ₆ H ₅ - <i>n</i> -C ₄ H ₉	134.2	1.40	-2.9	41.8	57.7

^a Computed, stoichiometric fuel-air mixtures at 1 atm pressure and 403 K unburned gas temperature.

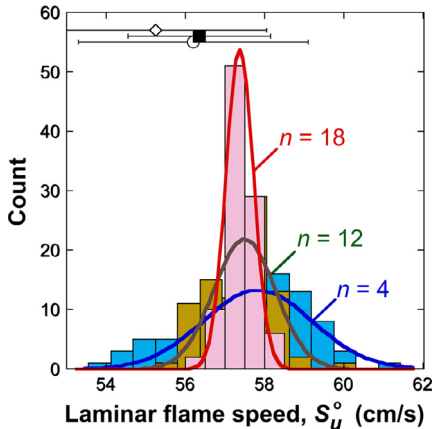


Fig. 1. Distributions of laminar flame speeds computed for 4-, 12- and 18-component Monte Carlo fuel mixtures in stoichiometric air at an unburned gas temperature $T_u = 403$ K and 1 atm pressure. Symbols are experimental data of Jet A (filled square), JP-8 (open circle), and JP-5 (open diamond) taken from Ref. [5]. The error bars on the flame speed data are 2σ standard deviations.

components to 57.4 cm/s at 18 components. Interestingly, these mean S_u° values are close to the flame speed values measured for real jet fuels, which range from 56.2 to 57.0 cm/s with a 2σ standard deviations of 2 to 3 cm/s.

A broader assessment of the effect of the number of fuel components on the high-temperature

combustion properties is presented in Fig. 2. The combustion properties assessed here are the ignition delay time (τ_{ign}) of stoichiometric fuel-air mixtures at three different conditions, atmospheric-pressure flame speeds from fuel-lean to fuel-rich mixtures, and the PSR extinction residence time (τ_{ext}) at 30 atm from fuel-lean to fuel-rich mixtures. It is seen that in all cases, the variations of the combustion properties decrease rapidly as the number of components increases. For two-component fuels, the ignition delay time varies by an order of magnitude, from 260 to 2600 μs for the stoichiometric mixture at $p_5 = 1$ atm and $T_5 = 1300$ K. The magnitude of the variation is nearly the same as the single component fuel (410 to 3400 μs at $p_5 = 1$ atm and $T_5 = 1300$ K, see Fig. S1 of SPM). In general, a two-component fuel mixture produces preferentially a reduced ignition delay time because the reaction of the slower reacting fuel component is typically accelerated by the faster reacting component. What is significant is that at 12 components, the 2σ standard deviation of the ignition delay time is reduced to $\sim 20\%$ or less, and that of the flame speed is around 2 cm/s or less, both of which are similar or smaller than the current measurement uncertainties for those properties. For fuels with 14 or more components, the variations in the combustion properties calculated become largely negligible in comparison to the accuracy of most legacy combustion chemistry experiments.

The results just discussed clearly support the principle of large component number introduced

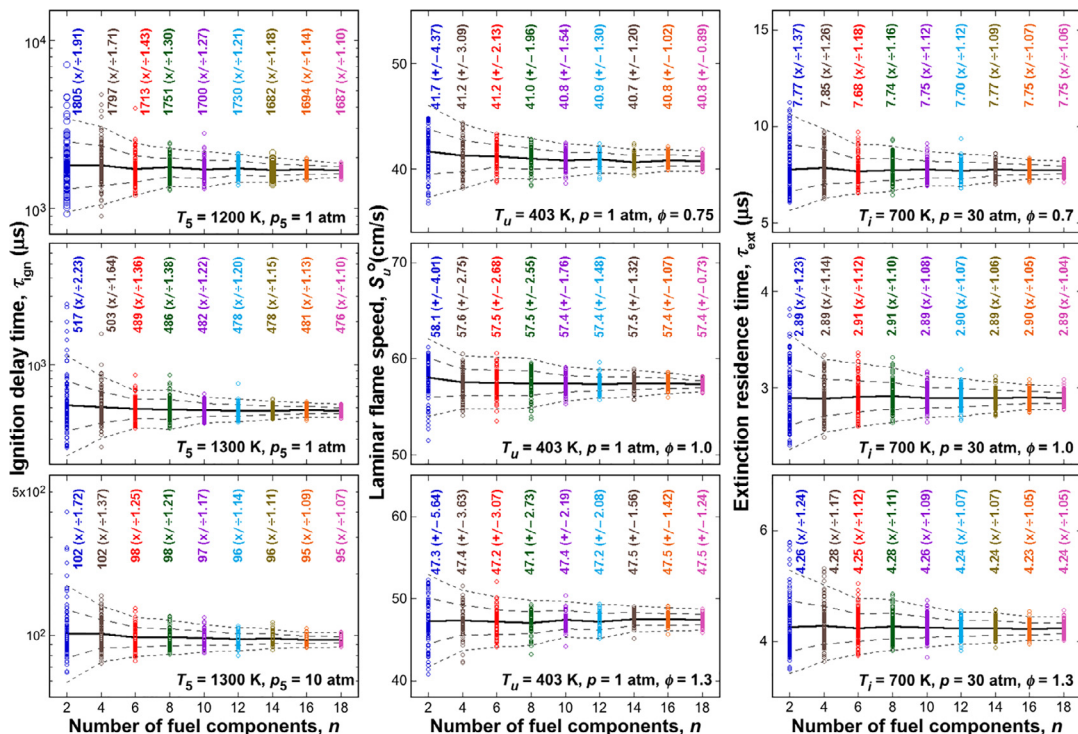


Fig. 2. Values of ignition delay time (left panel), laminar flame speed (center panel), and extinction residence time (right panel) computed for n -component fuel mixtures randomly sampled from Table 1 under the conditions indicated. The values in the figures are mean and 2σ standard deviation values. The solid lines are the mean values; the dashed lines are the 1σ standard deviations; the dotted lines are the 2σ standard deviations. Each set of calculations uses about 100 mixture samples.

earlier. Over the broader range of thermodynamic conditions and combustion phenomena tested here, basic combustion responses are insensitive to the fuel composition when the number of component becomes large enough. This and the past study [3] puts the critical number at about 12 to 14 components. Above this critical number, no shock tube, jet stirred reactor or flame apparatus is expected to discern statistical differences resulting from the variation of the fuel composition. In addition, the critical number appears to be universal across phenomena tested. The results also explain satisfactorily the previous observed insensitivity of shock tube ignition delay time to jet and rocket fuel variations [2] and of laminar flame speed over a wide range of conditions [5].

To explain the insensitivity just discussed, we examine the internal reaction processes focusing on the shock tube ignition delay. As discussed in recent studies [3,5], the high-temperature oxidation of large hydrocarbon compounds follows a process in which the fuel thermally decomposes first even with O_2 presence, followed by the oxidation of the pyrolysis products. The two processes are decoupled with the second, oxidation process being

rate limiting. To illustrate this behavior, we plot in Fig. 3 the time histories of n -dodecane (the fuel), C_2H_4 (the key pyrolysis product), OH (the key radical intermediate), and H_2O and CO_2 (the major products). The experimental data are taken from Davidson et al. [13]. The predictions are made with an unoptimized version of JetSurF 1.0 [14]. Our recent study has shown that the model can be optimized to closely reproduce the experimental time histories shown [15]. Regardless, both experimental data and model prediction demonstrate that under the conditions shown, fuel pyrolysis takes 20 μs , producing mainly ethylene (and other pyrolysis products not shown), but the ignition, as evidenced by the rapid rises in the CO_2 and OH concentrations occurs some 800 μs later.

Hence, the product distribution from fuel pyrolysis must be a major factor that determines the global oxidation rate. It follows that the insensitivity of the combustion properties to the composition of a multicomponent fuel must be related to the same lack of sensitivity of the pyrolysis product distribution to the composition of the fuel with a large number of components. Figure 4 shows the distributions of major products at 1 ms of

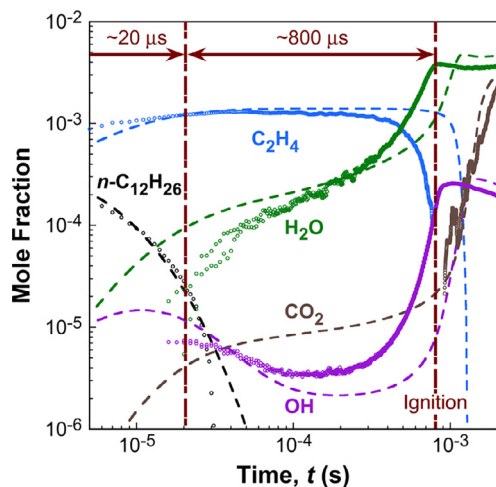


Fig. 3. Key species time histories of *n*-dodecane oxidation in a shock tube (475 ppm $n\text{-C}_{12}\text{H}_{26}$ and 7500 ppm O_2 in argon, $T_5 = 1410\text{ K}$, $p_5 = 2.15\text{ atm}$). Solid lines: experimental data [13]; dashed lines: simulation using JetSurF 1.0 [14]. The line dividing decomposition and oxidation is set at an arbitrary value of 95% fuel disappearance.

reaction time from the thermal decomposition, comparing the 4-component fuel mixtures to the 18-component fuel mixtures, in N_2 at 1300 K initial temperature and 1 atm constant pressure. The fuel mass loading is 6.3% in all cases, which is close to the mass fraction of a real fuel in stoichiometric air. Insofar as distillate fuels are concerned, key pyrolysis products are always the following eight species: ethylene (C_2H_4), hydrogen (H_2), methane (CH_4), propene (C_3H_6), 1-butene ($1\text{-C}_4\text{H}_8$), *iso*-butene (*i*- C_4H_8), benzene (C_6H_6) and toluene ($\text{C}_6\text{H}_5\text{CH}_3$), as discussed in Ref [3]. The current Monte Carlo analysis identifies the same species, as shown in Fig. 4, which account for over 80% of the carbon and hydrogen masses under the condition tested. Among these species, ethylene, propene, *iso*- and 1-butene are produced primarily from C-C β -scission of the hydrocarbon radicals; hydrogen and methane are from H-abstraction by H and CH_3 radicals; benzene and toluene are produced mainly from the decomposition of *n*-alkylbenzenes. Other species may include ethane (C_2H_6), acetylene (C_2H_2), propyne (*p*- C_3H_4) and allene (*a*- C_3H_4). They are produced from the secondary reactions of the key pyrolysis products listed above. Again, ethylene is almost always the most dominant pyrolysis product.

An inspection of Fig. 4 shows that the variations in the pyrolysis product distributions are rather broad for the 4-component fuel mixtures, but the thermal decomposition products of the 18-component fuel mixtures are narrowly distributed. Taking ethylene as an example, the distribution gives a mean mole fraction value of 0.0171 with

a 2σ standard deviation of 0.002, or $\sim 12\%$ variations. Suffice it to note that this level of variation is again smaller than the uncertainty achieved in the most advanced shock tube/laser diagnostics facilities (see, e.g., [5]). A minor finding from Fig. 4 is that for the 4-component fuel samples, *i*- C_4H_8 , C_6H_6 , and $\text{C}_6\text{H}_5\text{CH}_3$ are asymmetrically distributed towards zero. This is because extreme cases in a few-component fuel mixture are of a higher probability than a many-component one. These extreme cases are the cause for low or no aromatics or *iso*-butene production since benzene and toluene are produced almost exclusively from alkylbenzene and *iso*-butene comes mostly from highly branched *iso*-alkanes.

While in a statistical context the principle of large component number is similar to the law of large number, the phenomenon can be explained chemically. First, with the increase in the number of reactant components, the occurrence of extreme mixture compositions dominated by one or more extreme component is reduced by dilution. In a multicomponent fuel mixture, the more reactive fuel components would generate radicals over a shorter time scale than less reactive components. The less reactive components quickly scavenge these radicals, thus slowing the reactions of more reactive components. Conversely, the fast radical generation speeds up the reactions of the less reactive components. In doing so, the reaction processes become tightly regulated and tend to a converged state, so long as oxygen is involved in the decomposition process only to a limited extent. Additionally, global combustion properties, such as those studied herein, are mostly sensitive to the reactions responsible for radical chain branching and/or heat release. As long as the pyrolysis product distribution is relatively invariant, the rates of radical chain branching and heat release are also invariant. The aforementioned behaviors are, in fact, the fundamental reasons why combustion engines can tolerate the day-to-day, pump-to-pump, and region-to-region variations in fuel composition. We caution, however, that the principle should not be applied to the low-temperature and the negative-temperature-coefficient (NTC) regimes, as the chemistry in those regimes are sensitive to reactions that are fuel structure and composition dependent.

The chemical variations in the fuel mixtures sampled here are, in fact, larger than the variations seen in jet fuels. For example, the H/C ratios of conventional jet fuels typically vary between 1.85 to 2.00 [1], yet the 16-component mixtures sampled here have the H/C ratios ranging from 1.79 to 2.10. Additionally, it is known that in jet fuels, lightly-branched *iso*-alkanes with one or two methyl groups are much more dominant than highly-branched *iso*-alkanes [16]. Moreover, the weight percent of aromatics in jet fuels is typically less than 25% [1].

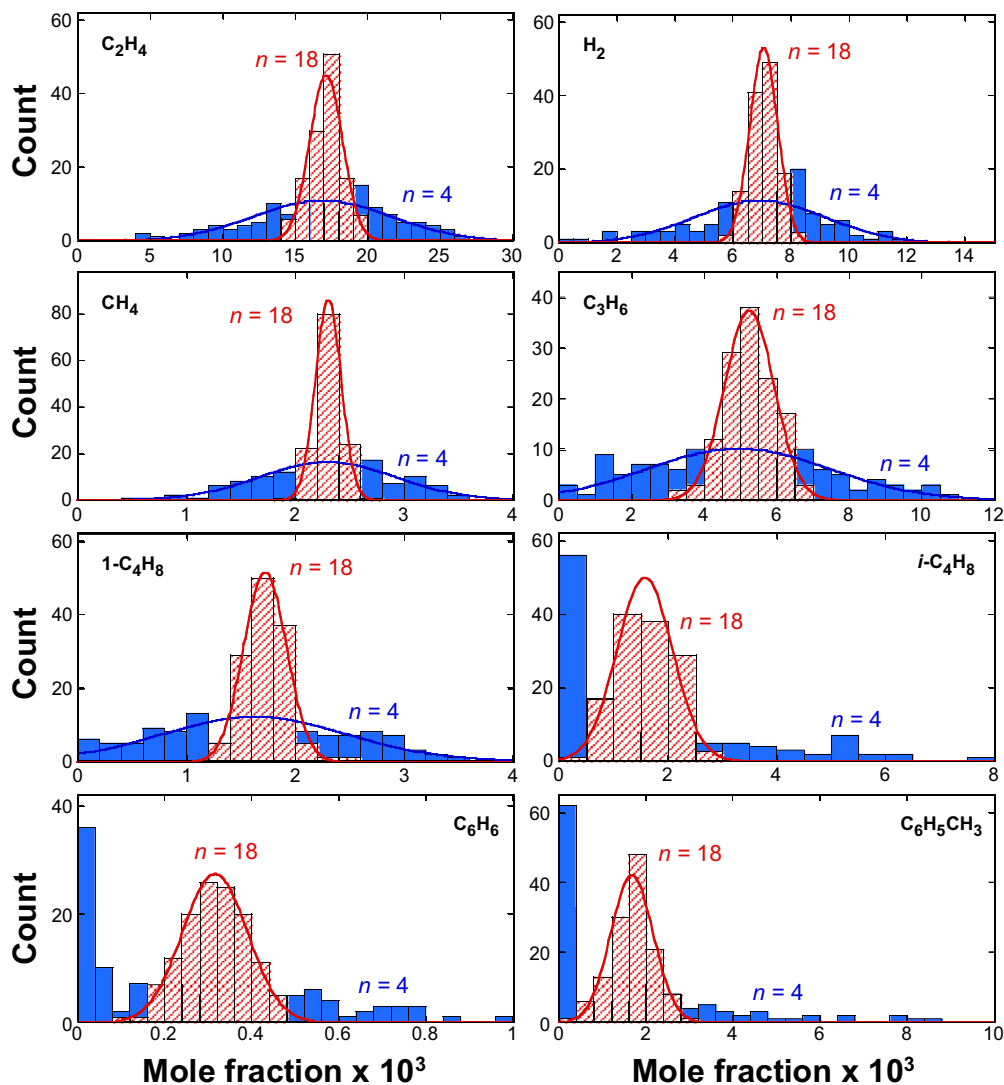


Fig. 4. Distributions of the major products computed for adiabatic and isobaric pyrolysis of 4- and 18-fuel component Monte Carlo samples. The initial conditions are 6.3 (wt%) fuel- N_2 mixtures, 1 atm pressure and 1300 K initial temperature.

To illustrate how the above constraints impact the variation of the fuel combustion properties and to better mimic the jet fuel physicochemical properties, we carried out constrained Monte Carlo samplings by creating a set of 128 16-component fuel mixture samples in which the H/C ratio is 1.95 ± 0.05 , LHV is 43.7 ± 0.2 MJ/kg, the mass fraction of aromatics is less than 25%, and lastly, *neo*-hexane and 2,2,4-trimethylpentane are excluded from consideration. The distributions of ignition delay time, laminar flame speed, and PSR extinction residence time are computed for these constrained fuel mixtures and compared to those of unconstrained fuel mixtures in Fig. 5. Not surprisingly, the 2σ variations are reduced with the

constraints. Also, with the constraints, the mean values of τ_{ign} and τ_{ext} are shifted towards shorter times, and the mean S_u^0 becomes larger, indicating that the constrained fuel mixtures are on average more reactive than the unconstrained mixtures. Excluding highly branched *iso*-alkanes enhances ethylene (C_2H_4) production and more importantly, reduces *iso*-butene (*i*- C_4H_8) production, thus increasing the mixture reactivity. As shown in Fig. 6, the *i*- C_4H_8 production from the pyrolysis of the 16-component fuel mixtures (6.3 wt% of fuel in N_2 at 1300 K, 1 atm and at 1 ms reaction time) is reduced by a factor of 4 on average.

The principle discussed herein has an important implication on surrogate fuel formulations.

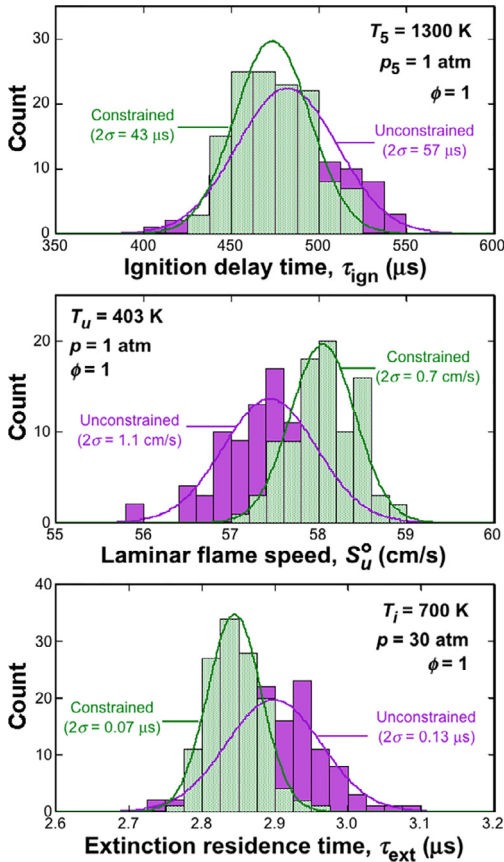


Fig. 5. Distributions of ignition delay time (top panel), laminar flame speed (middle panel), and PSR extinction residence time (bottom panel) computed for unconstrained and constrained 16-component fuel mixtures.

The widely adopted surrogate fuel approach [17–21] typically uses 6 or fewer number of hydrocarbon compounds, each of which represents a certain class of hydrocarbons in a real fuel. Together the mixture is expected to mimic the combustion behavior of a real fuel. Yet a few-component surrogate can hardly reproduce the distillation curve of a real fuel, at least not in a way that each distillate fraction can represent the homogeneity of the hydrocarbon classes as reported by Bruno and coworkers [22]. Hence, there is merit in increasing the number of components in the surrogate fuel so that both the chemical and physical properties of the real fuel can be reproduced. The fact that the key combustion behaviors are convergent for any fuel mixtures with more than 12 to 14 components and that the reaction models currently available are already sufficient to cover all major hydrocarbon classes found in real fuels suggests that future surrogate fuel research may have to consider the current findings as an integral part of its approach.

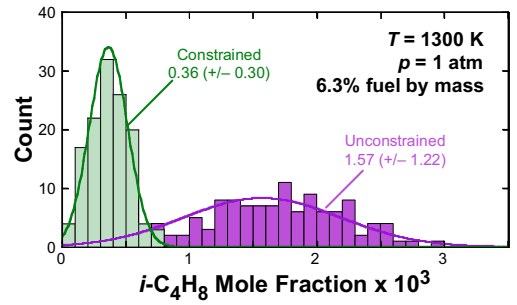


Fig. 6. Distributions of $i\text{-C}_4\text{H}_8$ computed for the adiabatic and isobaric pyrolysis of unconstrained and constrained 16-component fuel- N_2 at 1 ms of reaction time.

In fact, high-temperature combustion properties can be readily calculated with any of fuel mixtures having a critical number of components.

5. Conclusion

The principle of large component number is examined using Monte Carlo simulations. Fuel mixtures are formed by randomly selecting n ($n = 2, \dots, 18$) compounds from a group of hydrocarbons commonly identified in real distillate fuels. Ignition delay time, laminar flame speed, and extinction residence time in PSR are used as the test cases, covering a wide range of thermodynamic conditions and combustion phenomena. The results indicate that when the number of fuel components is larger than 12 to 14, the variations of any of the combustion properties vanish to a large extent. It is shown that with additional constraints imposed on the sampling to better mimic the real-fuel physicochemical properties, the variations in the combustion behaviors are further reduced. Lastly, we note that chemical kinetic modeling of multicomponent real fuels is not more complex than it has been perceived. While complexities do arise because of our inability to precisely define the fuel composition, the variation of the fuel composition is entirely unimportant because its effect on the combustion properties is small. To this end, the principle discussed herein should provide great simplification for quantitative analysis of the combustion chemistry of real fuels.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.proci.2018.06.187.

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