Characterizing Ignition behavior through morphing to generic curves

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Abstract

The qualitative notion that ignition processes have similar behavior, even over an extensive range of starting conditions, is quantitatively demonstrated through the production of a single 'generic' ignition curve. The key to the production of the generic curve is the recognition that the basic shapes of the species and temperature profiles occurring in the ignition process differ only in their 'timing'. By 'morphing' the time scale, the profile shapes can be made to align. From the aligned profile shapes a generic or 'average' profile can be derived. Synchronizing chemical events modifies the ignition progress times. In addition to fixing the ignition time to have the progress value of one, intermediate ignition events (such as selected profile maxima or inflection points) that occur before ignition are also aligned to have specific 'normalized' times.

Introduction[1]

Within a given parametric range (i.e. ranges of starting temperatures, pressures and equivalence ratios), which can be quite extensive, the behavior of an adiabatic homogeneous zero-dimensional constant volume (or pressure) process is quite regular. The process goes through several well defined regimes, for example initiation, build-up of radicals, ignition and finally equilibrium(Blurock, 2006, 2004). The curves in Figure 1 show that the behavior is similar, i.e. the curves look similar, regardless of the starting conditions(Griffiths and Barnard, 1998). The only real differences are when

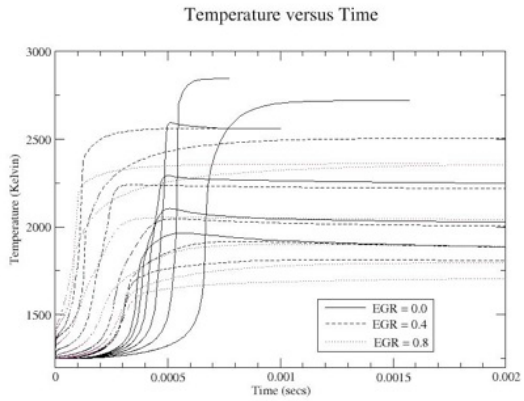

Figure 1: A set of ignition curves for ethanol at different starting conditions. The time versus temperature plot for 5 starting temperatures and three different equivalence ratios. The solid, dotted and dashed lines are for the equivalence ratios, 0.5, 0.75 and 1.0, respectively.

the events occur, for example ignition time, and exact values, for example the maximum values of species mass fractions. Exploiting these similarities is the basis of all kinetic reduction(Tomlin and Turányi, 2013). The prerequisite is that the mechanistic steps within the parametric range are similar. Within other ranges, with other mechanisms at work, another set, similar among themselves, of similar behavior would be observed.

Morphing to a single generic curve

A major purpose of this paper is to exploit the similarities of an ignition process to produce generic ignition curves, uniting ignition curves, each with different starting conditions, into one common behavior using one single progress variable. The inherent assumption is that a given progress value, regardless of its origin, should represent a given stage of the ignition process. In terms of species profiles, for example, this means that a given species reaches a maxima at the same progress value regardless of starting conditions. The creation of a single generic ignition curve (one for each species and two more for temperature and pressure) from a range of starting conditions is substantiation of the intuitive notion that the ignition process is going through the same set of mechanistic steps. Another range of parameters might represent another set of mechanistic steps and would be represented with another set of generic curves.

This paper, dealing with zero dimensional autoignition curves, performs a normalization process, similar to curve morphing (though usually associated with more complex objects (Alexa, 2002)) or conformal mappings (or a variety of other standard coordinate transformations). A transformation, through stretching and shrinking, of coordinates is used to produce a single generic curve valid under a range of conditions. The set of ignition curves, representing the temperature,

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pressure and mass fraction behavior of an ignition process, will be transformed to an average generic curve. This average generic curve is the quantitative representation of a combustion modelers intuitive notion of what is occurring within the combustion process.

The set of parameters needed to morph a specific curve to the generic curve is the basis of the parameterization of a given process. For example, there is a distinct and smooth relationship between ignition delay time and ignition starting conditions. This could be used as one of the bases of the parameterization of the curves.

A prerequisite to the production of a generic curve is to establish a new normalized progress parameter in which critical events before ignition are synchronized. This synchronization is necessary because the progress, usually defined by progress time to be the value of one at ignition, is non-linear, i.e. a specific ignition event under differing starting conditions does not occur at the same progress value. In this paper, not just one event is synchronized, such as ignition, is synchronized. Other events, such as the specific definable events on the curve, such as maxima, minima or inflection points, are also synchronized. An important consequence of this synchronization of chemical events is the ability to compare chemical behavior of the entire range of conditions at each transformed progress point. One such comparison is to take the average behavior at each progress point to form a single generic curve for each species. This single species curve represents the generic behavior of that species over the entire range of conditions. This generic behavior over the range of conditions can provide a generic characterization of the chemical processes involved in ignition. At a given progress value, the relative behavior of each of the individual intermediate species within the process can be compared. The process is basically characterized by one generic curve over progress time for each species.

In this paper, the ethanol mechanism of Marinov (Marinov, 1999), with 50 species, is used. This is a high temperature mechanism and the range of temperatures used in this study are from 1300 to 1400 Kelvin. In addition, this study is limited to lean (0.50) to Stoichiometric (1.0) mixtures.

Multiple Synchronizations

In many ignition parameterizations, a single progress variable is used to denote at what stage a process is, from initial conditions, with a value of zero, to the point of ignition, a value of one. In one sense, this can be viewed as normalizing or synchronizing the ignition processes under different starting conditions so that the ignition times line up. The single progress variable indicates the extent of the ignition process. When the ignition process of times of Figure 2 are normalized so that the point of ignition, defined by greatest increase of temperature, represent a progress of one, Figure 3 shows that the events leading up to ignition are not synchronized. For example, it is evident from the graphs that the maximum points of a given species, signaling a distinct event in the combustion process, do not occur at the same time under different conditions.

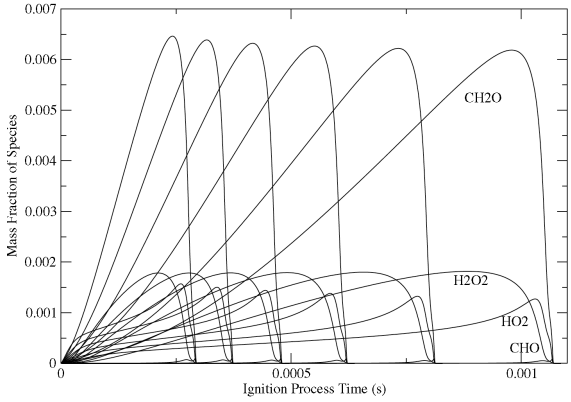

Figure 2: Concentration of select species without synchronization.

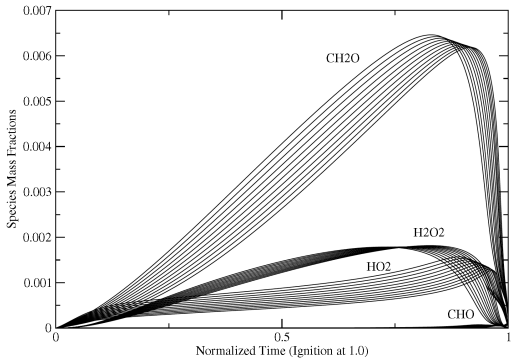

Figure 3: Synchronization of the curves of Figure 2 to have the ignition time defined at the same progress.

In the following sections, a transformation of the time progress will be made to 'actively' line up events within the ignition progress, so, at the end of the transformation, the time progress will represent a distinct phase of the ignition process. An ignition process goes through distinct phases. During these phases events occur, such as intermediate concentrations reaching a maximum or minimum, leveling off, increasing significantly and other recognizable functional features. These features, along with the time of ignition can also be included in the progress normalization process. In

other words, the process time is not just divided by a single factor, the ignition time, but is transformed or morphed in such a way that a set of specified events occur at the same progress value. At the end of this normalization process, not only are the selected events synchronized, but, indirectly, their associated events should also occur at the specific time progress values. The implication is that the progress time is not a steady linear relationship from reactants to ignition, but a non-linear one where, dependent on the initial conditions, given events deviate from linearity. To facilitate the automatic recognition of events, the ignition events are chosen as distinct features in the curvature of the species behavior, for example, maxima, minima in the values or in their derivatives.
The transformation is based on the intuitive notion that within a given range of conditions the chemical behavior within a process is similar. The human brain recognizes these similarities when examining the species behavior versus time curves of, for example, Figure 3. For example, the basic shape of the CH2O curves look very similar other than taken a different amount of time to reach its maximum and then fall again. The mathematical transformation of the progress time to ignition through morphing is a quantitative example of the similarity notion.
This paper sets up quantitative mathematical rules so that the similar events under different starting conditions, such as the rise and fall of the CH_2O mole fractions, are synchronized.
An important consequence of this synchronization of chemical events is the ability to compare chemical behavior of the entire range of conditions at each transformed progress point. One such comparison is to take the average behavior at each progress point to form a single generic curve for each species. This single species curve represents the generic behavior of that species over the entire range of conditions. This generic behavior over the range of conditions can provide a generic characterization of the chemical processes involved in ignition. At a given progress value, the relative behavior of each of the individual intermediate species within the process can be compared. The process is basically characterized by one generic curve over progress time for each species.
Figure 4 illustrates that with each additional time normalization the spread of the curves diminishes, even for a fairly extensive starting condition range. Even within each of the three difference equivalence ratio values, the curves are fairly synchronized.

Figure 5 shows that when the y-axis is synchronized, i.e. the maximum are all aligned, a single generic curve begins to emerge. This curve represents the general behavior and curvature of the ignition process.

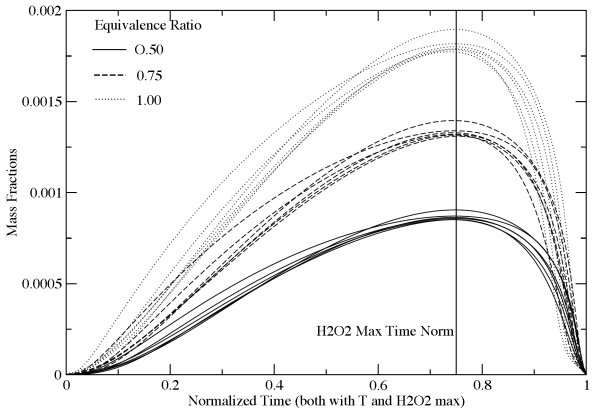

Figure 4: In this figure, both the ignition time and another event, the maximum of H2O2, are synchronized. It can be seen that

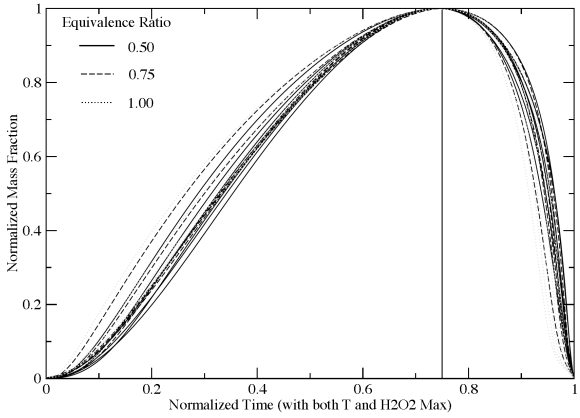

Figure 5: The single generic curve over all equivalence ratios emerges as the heights at the maximum are also aligned.

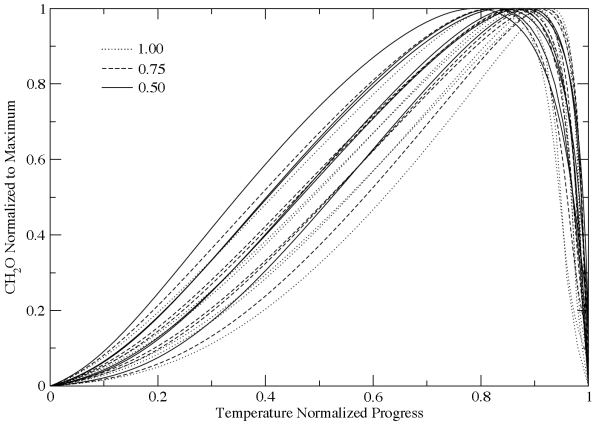

Figure 6

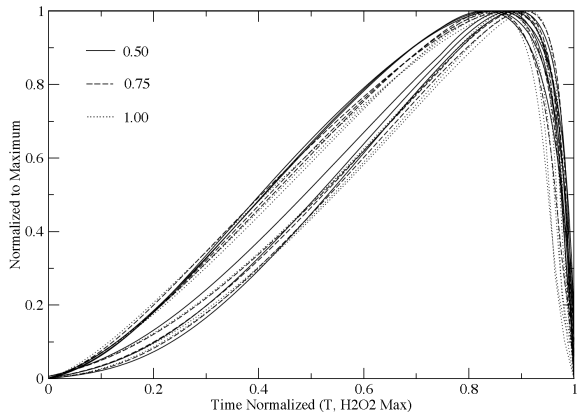

Figure 7

Though the synchronization with one extra event synchronizes that species of that event, it can be seen that indirectly, the remaining species, without explicit alignment, are also aligned. Figure 6 shows the CH2O curves with just the ignition aligned. With the extra synchronization of another species, as H2O2 shown in Figure 7, nevertheless the CH2O curves are brought closer together. Even though the time normalization does not directly involve the CH_2O species, the spread of the maxima is diminished with the addition of the normalization due to the H_2O_2 maxima. This effect is justified by the intuitive notion that the species in a combustion process are acting together, they are not independent of each other.

Range of validity and choice of events

A single generic curve is produced by morphing the individual curves to coincide at specified sequential chemical events. This is a mathematical description of the statement that the set of ignition curves have the same mechanistic chemistry. A combustion process undergoing a different set of mechanistic events should be described by a different generic curve. In this formulation 'a different set of mechanistic events' is defined as being a set of curves in which the set of chemical events occur and occur in the same order. This can be used as a criteria for differentiating combustion events with different mechanistic steps. A complete description of a combustion process over the complete set of ranges would be described by a set of generic curves.

The method is general enough to produce a generic curve for a given mechanistic process. The range of validity is in part determined by which chemical events one chooses to use as the basis of morphing. Using fewer chemical events to synchronize the timing of the processes could increase the range of validity, but this could be at the cost of crucial events not being synchronized.

The chemical events to be synchronized is partly a 'chemical' choice. One should choose those events that are crucial to the combustion process. This could either be done through chemical intuition or even through active methods such as, to name one, sensitivity analysis. There is, however, a 'mathematical' criteria. The synchronizing event has to able to be mathematically recognized, for example a maximum, minimum or point of inflection must occur in the combustion process. There is also an additional 'coverage' criteria. The set of synchronizing events should be representative of the different combustion mechanisms that occur within the combustion process (for example the different chemical regimes found by clustering in the paper of (Blurock, 2006, 2004)). In other words, the chosen events should span the entire combustion process being described. Some chemical 'events' can be described by two parameters, for example, both parameters reach a maximum at the same time. Using both parameters would be redundant.

In this paper a zero dimensional process over ignition time has been chosen as the example. But the method itself is purely mathematical and not restricted to only ignition processes. For example, one dimensional flames could be also be described bygeneric curves. The primary criteria to apply the method described in this paper is that a multivariate event is described by a single variable 'progress'. The example in this paper should be thought of a 'proof of concept', that indeed the synchronization of events does occur and consequences of these synchronizatons can be seen.

Conclusions

The intuitive notion that combustion processes within a given range of conditions representing similar mechanistic steps is quantitatively justified with the concept of generic curves over a single parameterization.

The generic curves are produced by synchronizing not only the point of ignition, but a choice of chemical events before ignition. These chemical events can be automatically recognized by distinct mathematical features, such as maxima, minima or inflection points.

Acknowlegements

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