

Characterizing Ignition behavior through morphing to generic curves

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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. With this additional synchronization, a single generic curve, derived from the average of the morphed curves, can be derived. This generic curve represents a kinetic modelers intuitive notion of the mechanism of the process.

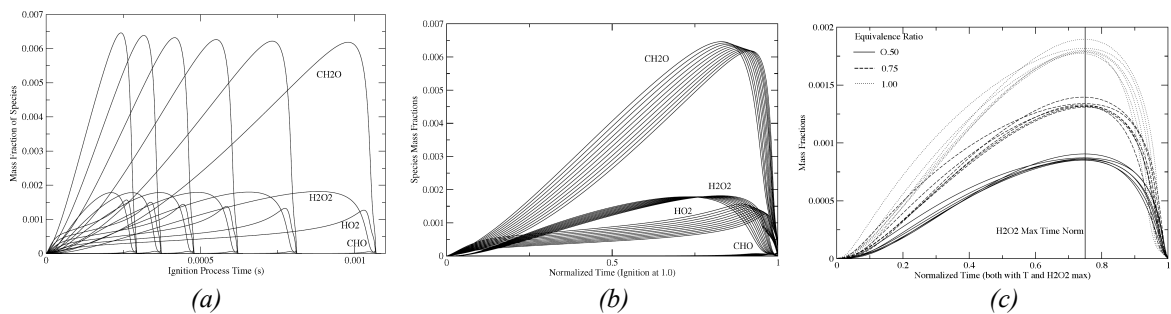


Figure 1: Three concentration profiles with the original progress (a), normalized with just the ignition progress (b) and finally with the H_2O_2 maximum also synchronized

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.

If the mechanistic pathway is similar for a set of starting conditions, then the set of fixed synchronization points exist and occur in the same relative order. If the mechanistic pathway differs, then the synchronization points change order, may not exist or there are others. Thus the set of synchronization points can be criteria for differentiating different mechanisms.