Steady State Reduced Mechanisms based on Domain Splitting

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The Quasi Steady State Assumption (QSSA) reduces the computational effort within a mechanism by identifying steady state species, By automatically recognizing different reactive domains within a chemical process using a machine learning clustering technique, a further reduction of a mechanism's computational complexity is achieved. The requirement that a species be in steady state for the whole process is relaxed to having only to be in steady state for one of the domains in the process. This results in more species, in total, being in steady state creating a total reduction of the mechanism's complexity. In this paper the steady state species is identified by criteria based on a level of importance factor (LOI) involving species sensitivity and lifetimes. The method is applied to calculations of ethene diffusion flame.

1 Introduction

The Quasi Steady State Assumption (QSSA) reduces the computational effort within a mechanism by identifying species, steady state species, whose source terms can be solved algebraically instead of solving their associated differential equation. In previous work[1], steady state species were identified by criteria based on a level of importance factor (LOI) involving species sensitivity and lifetimes. If a species meets this criteria throughout the entire process, then that species is defined as steady state throughout the entire process.

Within a complete combustion process there are reactive domains of differing chemistry and physics. Different reactions and species are important in different domains. The steady state species within each domain could be different. In addition, a given species could be in steady state for one domain, but not for the entire process. The current method takes advantage of this by defining steady state species with respect to domains instead of the entire range. The relaxed criteria allows more species to be defined as steady state. The result is a reduced computational complexity.

The key to this improvement is the automatic identification of the chemical domains through clustering. Clustering, in general, identifies objects which are similar by a given criteria. If the criteria is a measure of reactivity, then a cluster would be a domain of similar reactivity. In this work, similar reactivity means that the same set of species are in steady state. A clustered domain would mean that the same set of species are in steady state throughout the domain.

The main focus in this paper is the reduction of chemical mechanisms by the identification of chemical domains.

2 Method

In this study a counterflow flame is modeled with ethene as the fuel. The chemical mechanism in this study is a C_4-mechanism with 81 species and 806 reactions. It was originally derived by Chevalier et al. [3] and developed

further by Mauss for treatment of fuel rich flames and soot formation. The mechanism is treated using the flamelet model[2].

The foundation of the proposed method is a machine learning cluster method[4] which, in general, takes a set of objects and clusters them into groups of 'similar' objects. In this paper, there is an object at each mixture fraction of the stationary flame solution. Each mixture fraction is described by a vector of LOI values. Each cluster defines a domain and is a range of mixture fractions. Thus the similar reactivity within a domain is when the set of steady state species are the same or similar.

In the determination of steady states, a user-set cutoff value is used to determine whether a species is steady state or not. In the clustering method, instead of using the LOI value itself, the state description of each object is a 'fuzzy' predicate on the LOI value asking whether the species is in steady state or not. A fuzzy predicate is used to make the transition smoother. In other words, around the cutoff, a species can have partial steady state character.

The reduction of the mechanism occurs in two stages. First, in a preprocessing step, the domains are identified through the clustering method described. Within each domain, the set of steady state species are identified using the same cutoff level that was used in the clustering procedure. During the calculation, the steady state species are calculated through a numerical steady state procedure by neglecting diffusion and convection terms in their balance equations. In this study, it is assumed that there are no discontinuities, especially in the species concentrations, between domains.

The emphasis in this study is to compare the reduction achieved by varying the clustering level and the LOI cutoff value. As the cluster level increases, so does the number of clusters. Varying the cutoff value increases the number of species in steady state.
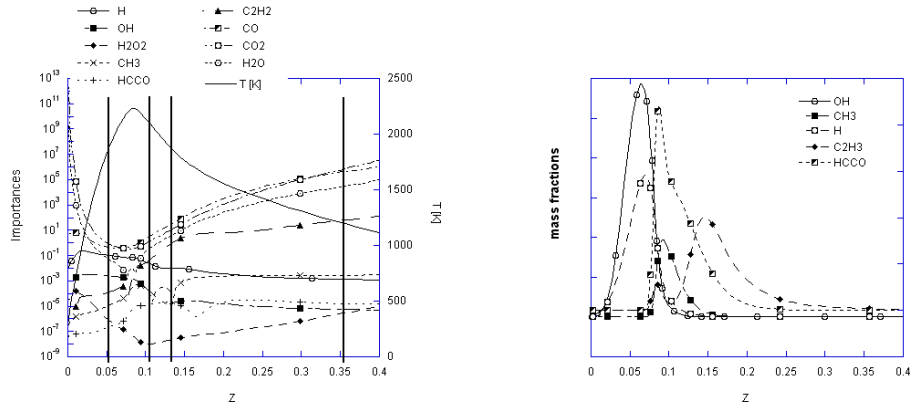

Figure 1: This figure illustrates the automatically derived cluster domains (whose bounds are the vertical lines). The first graph is mixture fraction versus LOI values for various species giving an indication of why the clusters were formed. The second graph shows mixture fraction versus mass fractions of several species.
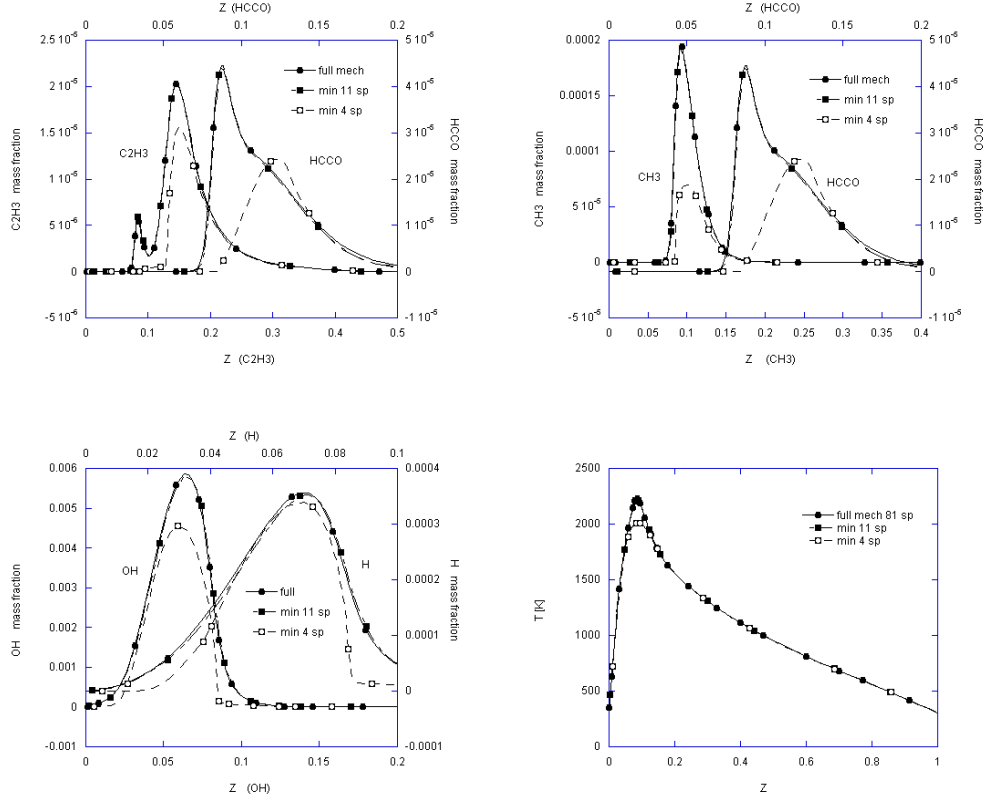
Figure 2: The accuracy of the species profiles as a function of the mixture fraction for some selected steady state species using reduced mechanisms with increasing degree of reduction. The mechanisms are denoted with their number of species in the most reduced domain.

3   Results

By varying the LOI cutoff value, mechanisms with different degrees of reduction can be achieved. Figure 2 illustrates the accuracy of the species profiles for different reduction levels as a function of the mixture fraction. The results from employing the reduced mechanisms are compared with that from employing the full (non-clustered) mechanism. From the figure it can be concluded that reduced mechanisms with a minimum number of species of 11 species performs very well, whereas a reduction to a minimum of 4 species is revealing some discrepancies in the species profiles and the temperature profile in the reaction zone. In this case, even the OH, H and other important radicals are set to steady state, thus introducing an error in the calculations of their concentrations. This in turn is closely related to the error in the temperature profile. The same type of discrepancies is also visible for the other selected steady state species. However, the trends are reproduced well by the very most reduced mechanism.

As seen from table 1, a single domain (i.e. no clustering) represents the same number of species as the maximum number in any of the other cases with several domains. In fact, most of the other domains are considerably less. This indicates the advantage of applying the cluster method to eliminate as many species as possible

Size	Domain	Range	Species
1	1	0.00 - 1.00	37
3	1	0.00 - 0.04	8
	2	0.04 - 0.10	4
	3	0.10 - 0.13	5
	4	1.13 - 1.00	37
5	1	0.00 0.06	8
	2	0.06 0.10	4
	3	0.10 0.13	6
	4	1.13 0.36	15
	5	0.36 1.00	37

Table 1: The effect of cluster level is shown on the domains found. *Size* is the number of domain, *Range* is the mixture fraction range for each *Domain* and *Species* is the number of non-steady state species.

within the domains. It is worth noting that in the fuel lean region of low mixture fractions, even the fuel can be set to steady state. This would not be possible for a single zone situation. The domain representing the fuel-rich side where the chemical lifetimes are long is found to give the lowest number of steady state species. This is a consequence of the large number of stable species with high concentrations and long lifetimes. A stronger reduction in the region is still possible if the LOI is normalized in a proper manner. From figure 1 the trend is clear that the values increase several orders of magnitude towards the fuel rich region compared to the values in the reaction zone where the general chemical lifetime is much shorter. Thus in future work a properly normalized value of LOI is believed to bring down the number of species in the colder outer regions.

References

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