

COMPARISON OF AUTOMATIC REDUCTION PROCEDURES FOR IGNITION CHEMISTRY

T. LØVÅS,¹ P. AMNÉUS,¹ F. MAUSS¹ AND E. MASTORAKOS²

¹*Department of Combustion Physics
Lund Institute of Technology
P.O. Box 118*

S-22100 Lund, Sweden
²*Department of Engineering
University of Cambridge
Cambridge CB2 1PZ, United Kingdom*

In this paper, we present a comparison between the reduced mechanisms obtained through a computational singular perturbation method (CSP) and the reduced mechanisms obtained through a lifetime analysis based only on the diagonal elements of the Jacobian matrix and a species sensitivity. The two methods are used for the analysis of autoignition, which is an interesting test situation because of the sensitivity of ignition to the radical pool and the smaller range of timescales expected. It is found that the steady-state species selected by the two methods are in good agreement. The mechanisms are reduced to a 10-step mechanism when CSP is applied and an 11-step mechanism in the case of the simpler lifetime analysis. Both mechanisms are compared with the detailed mechanism and experimental data and are found to reproduce the physical and chemical parameters very well. This shows that for a large part of the timescale range, the system is close to linear. The comparison shows the advantage of the CSP method as being somewhat more accurate. However, the simpler lifetime analysis is of sufficient accuracy and of more convenience when applied to a system requiring a considerable reduction in computational time, as is the case when applying *online* reduction.

Introduction

The motivation behind the development of methods for automatic reduction of chemical mechanisms is the demand for a speedup in computational time for complex simulations of combustion phenomena. By reducing the number of species that need to be modeled in detail, the overall CPU time and memory requirement is considerably reduced, since the number of differential equations that need to be solved is reduced. For the most complex systems, as for a computational fluid dynamics computation (CFD), a reduced mechanism is not an option but a necessity. In this case, an *online* reduction procedure is of convenience [1] where species are reduced at each computational step according to the physical conditions at that particular point. This results in a most efficient reduction procedure. To achieve this, a very fast reduction procedure is necessary and the accuracy of such a method is tested in this paper by comparison with a fuller approach based on the computational singular perturbation (CSP) [2–7].

The starting point of any reduction is a detailed or a skeletal mechanism. The mechanism is reduced by applying a chosen reduction procedure that can exclude species from the mechanism, or rather detect the species that can be described by approximate

means. Depending on the complexity of the physical system, mechanisms with an increasing degree of reduction can be applied. The main assumption underlying the application of the quasi-steady state (QSSA) is that many of the chemical processes occur on timescales much smaller than the physical processes, and these can be described in approximate terms without loss of accuracy or important information. When a species is set to steady state, the species source term is simply assumed to be zero, thus replacing the differential equation describing the species conservation equations with an algebraic equation. The success of the method depends on a reliable procedure for determining the species that are involved on the shortest timescales. The procedure is further optimized by determining the species that are of little importance for the accuracy of the results and which can thus be assumed to be in steady state without loss of important chemical information.

Several methods have been introduced and applied with success for a variety of applications. The methods that are of most interest are the method of intrinsic low-dimensional manifolds (ILDM) [8], the computational singular perturbation method (CSP) [2–7], and the lifetime analysis based on the chemical lifetime and QSSA [9]. The first method applies

a tabulation method for large amounts of data connected to concentration manifolds. These contain information about the chemical equilibria in the form of concentration values as functions of a chosen progress variable. These tables are applied in run-time, saving computational time. This tabulation procedure is different from that of the two other methods noted above and which are the methods to be considered here. They perform an analysis to detect steady-state species and thereafter apply the QSSA in order to reduce the set of differential equations governing the chemistry. This results in a considerable saving of CPU time.

However, the two methods apply different procedures in order to detect the steady-state species. The basis of the CSP method is to describe the set of equations governing the chemistry by a set of basis vectors. The problem becomes an eigenvalue problem where *fast* modes can be discarded from the *slow* modes. Steady-state species are thereby those species involved in the fast modes only. The lifetime analysis based on the chemical lifetime makes the assumption of a diagonal Jacobian meaning that coupled timescales are not accounted for. The diagonal elements of the Jacobian matrix are easy to compute in run-time and are used as a representation of the chemical times. The assumption of a diagonal Jacobian matrix is valid for the very shortest timescales. However, in the upper range of the timescale, the non-linear effects become more prominent.

It is believed that the CSP method is a more thorough method accounting for the physical and chemical conditions that are present with a higher precision than the simpler lifetime analysis when applied to a single reduction procedure. However, the method of generating the eigenvalues as described above is still found to require considerable CPU time and is not practically applicable when implemented as part of an *online* reduction method for speedup of the calculation [1]. In this case, the lifetime analysis based on the chemical lifetime is more appropriate.

In this paper, results from both methods are compared for an autoignition process. This particular process is chosen as a test situation because of the sensitivity of ignition to the radical pool and the smaller range of timescales expected compared with, for example, flames. This is of particular interest in terms of the direct comparison of the result from applying the reduced mechanisms originating from the two methods, and because the methods have not been validated before for ignition. This comparison also shows the advantages and disadvantages of applying the respective methods in a very direct way and will be a useful guide for future development and application of the methods.

This paper is organized in the following way: The first section briefly discusses the physical and chemical system. The discussion then progresses to outline the CSP methodology. Thereafter, the underlying formulation of the lifetime analysis based on

the chemical lifetime is presented and validated for ignition. This is followed by the validation and results from applying reduced mechanisms of varying degrees compared with the detailed mechanism. Finally, the conclusions are presented.

Physical and Chemical Modeling

The physical system chosen is a test case simulating a homogenous autoignition process. The system is described by the set of conservation equations governing species mass, momentum and energy predicting the evolution of the reactive mixture, and the physical parameters. The equations governing the physical system can be studied in Ref. [10].

The chemical kinetic model used for this work is a detailed C₁–C₂-mechanism under development. The mechanism consists of 46 species and 467 reactions intended for formaldehyde, methane, and methanol combustion over a wide range of operating conditions. The chemistry for H₂–O₂–CO–CO₂ combustion originates from Yetter et al. [11]. Remaining reactions and their rates are compiled from various sources.

In order to compare the performance of the reduced mechanisms, with the detailed mechanisms, the resulting ignition times, τ , are investigated under various conditions. The ignition is defined as occurring where the temperature gradient is at its maximum, that is:

$$\tau_{\text{ign}} = \tau|_{\max(\partial T/\partial t)} \quad (1)$$

The results for validation of the methods are obtained under constant pressure, and fueled with methane and air at stoichiometric equivalence ratio. When studying the agreement between the reduced mechanism, the detailed mechanism, and the experimental data, the methods are applied to simulations operating under constant volume fueled with a mixture of methane, argon, and oxygen to a mixture of equivalence ratio $\Phi = 0.75$ to correspond to experimental data. The calculations were performed accordingly for the verification versus the shock tube experiments by Spadaccini and Colket [12]. In the experimental data, the ignition delay time is monitored by two procedures. One procedure analyzed the pressure rise in the tube. The other method measured the emissions of OH and defined the ignition delay time to coincide with the maximum OH present. This definition is found to be almost identical to the definition given in equation 1.

The CSP Analysis

The CSP method has been described in the past in Ref. [6] and in references therein. Essentially, CSP calculates the eigenvalues of the Jacobian matrix of the source term and then identifies the species

that are mostly related to these. This is achieved by the "CSP pointer," which is a local quantity. To construct global mechanisms, the CSP analysis is performed in a selected region of the calculation domain (in space or time), and the local CSP pointers are weighted by the local production rate (normalized by its maximum value in the domain) and divided by the local species mole fraction. This weighted pointer is then integrated across the domain of interest. The weighting procedure has been discussed in Ref. [6], where other weighting factors were also tested. The one used here has been shown to be the more robust, that is, to give the best global reduced mechanisms. An ordering of these integrated pointers then shows which species can be taken as steady state (the ones with high values of the integrated pointer) or as major species (the ones with low values). The procedure has been discussed at length in Ref. [6] and its usefulness for constructing various reduced mechanisms and for yielding insights to the chemistry in Ref. [7]. The purpose is to construct as accurate global reduced mechanisms as possible based on local analyses.

In this paper, we use the same procedure, but to an autoignition problem. We use time traces of the species mass fractions up to the point of ignition and, based on the local CSP pointers at each time instant, the integrated CSP pointers are ranked, and a global reduced mechanism can then be defined. Reduced mechanisms with 20, 15, 11, and 10 global steps for methane autoignition have been successfully constructed here, and the results are compared with the lifetime analysis species selection method, outlined next.

The Lifetime Analysis and Calculation of the Level of Importance

In a homogeneous system, the chemical lifetime for a single species can be estimated from the Jacobian matrix. It can be shown that the diagonal elements, J_{ii} , are measures of the rates of readjustment toward equilibrium after a concentration perturbation, with a corresponding chemical lifetime ϑ_i^C given by

$$\vartheta_i^C = -1/J_{ii} \quad (2)$$

This lifetime includes only the diagonal elements of the Jacobian matrix without accounting for any coupling between the timescales. Strictly speaking, this is not the case; but it is, however, shown to be a good approximation for the shortest timescales which will be important for selecting the steady-state species [13]. The lifetime quantity is easy to extract in run time, and can be calculated by postprocessing the solution without introducing any noticeable additional numerical effort. The Jacobian diagonal can be obtained by differentiation of the chemical source

term with respect to the species concentration. Thus, the chemical lifetime is calculated as

$$\vartheta_i^C = -1 / \left(\frac{\partial \omega_i}{\partial c_i} \right) = \frac{c_i}{\sum_{k=1}^{N_R} (v'_{ik} - v''_{ik}) v'_{ik} r'_k} \quad (3)$$

where ω_i is the species source term, c_i is the species concentration, v_{ik} is the stoichiometric coefficient, prime denotes the reactant values, and double prime denotes the product values. The consuming reaction rate is r_k for individually treated reactions with the reaction coefficient k_k using the Arrhenius law. The forward and backward reactions are treated separately; consequently, for species not being an inert third body species, the stoichiometric coefficient on the product side is equal to zero if the stoichiometric coefficient on the reactant side is non-zero. One should note that ϑ_i^C is a local quantity, and that equation 3 may also be used for non-homogeneous cases, for example, flames. In the previous publications of some of the current authors, this chemical lifetime has been normalized to a selection of physical parameters that strongly influence the species concentrations such as the diffusion process and the convective time in flames [14]. In the present homogeneous case, these normalizations are not performed for obvious reasons and the above-mentioned representation of the chemical lifetime is used throughout the paper. The construction of global mechanisms will be discussed below.

If a species is selected for elimination by QSSA using a maximum limit for the lifetime measure together with a limit for the maximum concentration and/or species enthalpy of this species, a code-generation procedure like the one described in Ref. [15], excluding the reaction flow and sensitivity analysis, can be used for fully automatic generation of a reduced mechanism. The species with values lower than a specified cut-off limit are then selected for being set to steady state and the new reduced mechanism is automatically written as source code.

When applying the QSSA reduction method, it is important to bear in mind that an error is introduced into the system. The error originates from the approximations of the steady-state species concentrations. The absolute error introduced to the profile of an unknown j , f_j , by the error in the steady-state species profile of species i , f_i , is given by

$$f_j = \frac{\partial c_j}{\partial c_i} f_i + \sigma (f_i^2) \quad (4)$$

where the first factor on the right-hand side represents a sensitivity of species j toward species i . By applying the chemical lifetime as a selection parameter for steady-state species, it is assumed that the chemical lifetime is proportional to the relative error f_i , as given above. Only then is the selection based

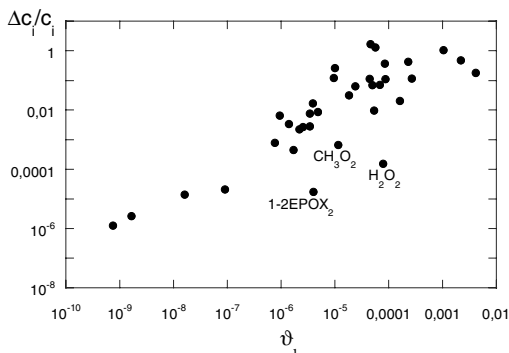


FIG. 1. The calculated error in relative concentration profiles as a function of chemical lifetime. The error is found by individually setting species to steady state and comparing the resulting maximum concentration with the maximum concentration obtained from a full calculation.

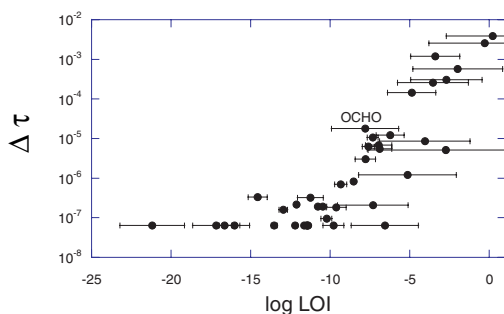


FIG. 2. The calculated error in ignition timing profiles as a function of LOI. The error is found by individually setting species to steady state and comparing the resulting ignition delay time with the ignition delay time obtained from a full calculation. Error bars for the calculated LOI are included illustrating the proportionality between the imposed errors and the species LOI.

on the chemical lifetime reliable in the sense that species introducing an overly large error into the system are not set to steady state. It is of most importance to investigate this proportionality given as

$$\frac{f_i}{c_i} \propto \vartheta_i^C \Rightarrow f_i \propto c_i \vartheta_i^C \quad (5)$$

Figure 1 is based on an investigation of the validity of equation 5. The calculated error in the concentration of species i is found by setting species i to steady state and comparing the resulting maximum concentration with the maximum concentration obtained from a full calculation. The species are set individually to steady state for each run, that is, one species at a time. The notation f_i is the predicted value, whereas $\Delta C/C$ in Fig. 1 denotes the relative calculated value.

In Fig. 1, this proportionality is shown to be valid up to the upper range of the chemical lifetime. This is when the non-linear effects become important and the spread of the values is noticeable. Some species are still lying off the main diagonal with the result that these species will not be properly selected as steady state, although they introduce lower errors than other species with the same lifetime. However, the tendency is clearly that the errors are monotonously increasing with lifetime.

In previous investigations by some of the authors using the pure lifetime quantity or a mass-fraction-weighted version, fully automatic QSSA reduction was possible to a certain extent only, resulting in mechanisms for ignition of four-component natural gas with the number of non-steady-state species still amounting to 20 [16]. Some species with a short lifetime need to be kept in the mechanism in order not to introduce too large an error into the system. On the other hand, species with a low sensitivity on the desired result, for example, flame speed or exhaust gas emissions, are still automatically kept in the mechanism due to long lifetimes. A larger error is acceptable in the equation for this species. Hence, in order to make the selection procedure more efficient, species with long lifetimes and low sensitivity should be eliminated, and the reduced reaction mechanism would be more suitable for use in CFD calculations.

To include the species sensitivity in the selection procedure the following parameter, the level of importance (LOI), is introduced and investigated in order to detect steady-state species [14]:

$$\text{LOI}_i \equiv S_{x,i}^S c_i \vartheta_i \quad (6)$$

where $S_{x,i}^S$ represents the species sensitivity of a parameter x on species i . This selection parameter is based on the same arguments put forward above and the fact that an error introduced to a chosen parameter x in the system, f_x , resulting from a relative error in the profile of a steady-state species i , f_i is given by

$$f_x = \frac{\partial x}{\partial c_i} f_i + \sigma(f_i^2) \quad (7)$$

The first factor in the first term on the right-hand side should be recognized as the species sensitivity of the chosen parameter on species i , $S_{x,i}^S$, and the second factor, f_i , is proven to be proportional to the chemical lifetime. In the ignition case, the interesting parameter for the species sensitivity is the ignition timing. For details on the sensitivity analysis, see Ref. [15].

According to equation 7, the absolute error in the ignition timing introduced by an error in the profile of a steady-state species i is proportional to the LOI as defined in equation 6. Fig. 2 shows an investigation of the validity of equation 7. The error is found by individually setting each species to steady state

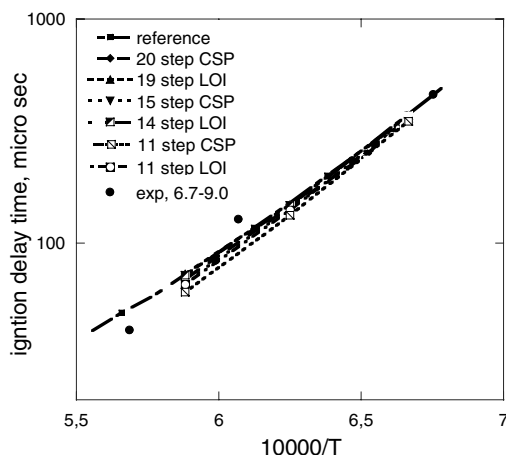


FIG. 3. Ignition timing as a function of inlet temperature shown for the inlet pressure of 7.8 bar. Results from a simulation with the detailed mechanism is validated against experimental data and is compared with the values resulting from the reduced mechanisms.

TABLE 1
Major species left in the 10-step mechanism from both CSP and lifetime analysis

Ten-Step Mechanisms	
CSP	Lifetime Analysis
OH, OCHO, CH ₃ CHO	CH ₃ , C ₂ H ₂ , CH ₃ OH
C ₂ H ₆ 1500K, O _{1600-1700K} , H _{1538K}	C ₂ H ₆
CH ₃ CO	CH ₃ CO
CH ₄	CH ₄
CH ₂ O	CH ₂ O
C ₂ H ₄	C ₂ H ₄
H ₂	H ₂
CO	CO
H ₂ O	H ₂ O
O ₂	O ₂
CO ₂	CO ₂
Ar	Ar
N ₂	N ₂

For CSP, the 10-step mechanism varies slightly according to inlet temperature. The subscript denotes the inlet temperature where the species is kept in the mechanism.

and comparing the resulting ignition time with the ignition time obtained with the full calculation. The notation f_x is the predicted value, whereas $\Delta\tau$ in Fig. 2 denotes the calculated value.

The absolute error in the ignition timing monotonously increases with LOI. Thus, selected steady-state species will not introduce a higher error into the computation than accepted from the respective

LOI chosen as a upper limit for steady state. Some non-linear effects are still visible in the upper range of the LOI. However, the results show an improvement from applying only the chemical lifetime and will be used as a selection parameter when developing reduced mechanisms for application in the simulations of ignition processes presented below.

Some species lie off the main diagonal as seen also in Fig. 1. However, since, according to the error term in equation 7, the error is a function of f_b , which in turn is proportional to the lifetime, it is found that the species lying off the diagonal are the species with a long lifetime and have accordingly a higher error in their LOI. The species in question are found to be the stable species. These error bars are included in Fig. 2, and if account is taken of the errors in the LOI, the selection parameter is shown to be consistent and reliable. The absolute error in the ignition timing increases monotonically with LOI.

Results and Discussion

For a chosen mixture, inlet temperatures were varied between 1500 and 1700 K for an inlet pressure of 7.8 bar. The resulting ignition delay times are recorded and the results from simulations using mechanisms with increasing degrees of reduction are compared with the detailed mechanism and the experimental data. Fig. 3 shows ignition delay times as a function of the inlet temperature for the same inlet pressure of 7.8 bar. It is clear from the figure that the reduced mechanisms obtained both from applying CSP and lifetime analysis are in good agreement with the detailed mechanism and the experiments down to the most reduced mechanism. An 11-step mechanism developed from CSP analysis performs equally well as the 11-step mechanism obtained by using the LOI. In the case of applying CSP, ignition was obtained even for a 10-step mechanism. However, the error introduced to the system becomes significant for such a reduced mechanism and it is not included in the figure. The reduced 10-step mechanism obtained from LOI did not predict ignition within 10 ms and is considered as non-igniting. Thus, an advantage is shown in using CSP for finding species in quasi-steady state. The selection of steady-state species is more consistent if the eigenvalue problem is solved.

It is of interest to investigate the difference in the resulting mechanism after reduction to 10 steps. The CSP method provides different mechanisms for different inlet temperatures. When applying the lifetime analysis, the LOI is integrated over time until the ignition criterion is reached, and maximum values over the range of inlet temperatures are applied. Table 1 shows the remaining species after application of the two different methods. The species that are kept in the reduced mechanism by applying CSP

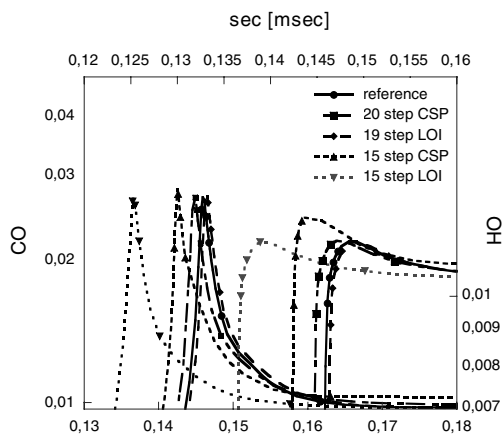


FIG. 4. CO and OH profiles resulting from reduced mechanisms with increasing levels of reduction compared with the result of applying the detailed mechanism.

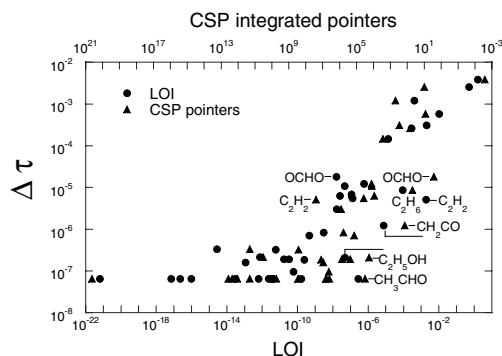


FIG. 5. The error in ignition-timing profiles as a function of integrated CSP pointers compared with LOI. The results are obtained in the same manner as for Fig. 2.

that are not retained in the mechanism resulting from the lifetime analysis are OH, OCHO, and CH_3CHO . These species together with the remaining species are responsible for the onset of ignition as no ignition is obtained without them.

It is also important that the mechanisms can reproduce the concentration profiles of important species. The error introduced in the ignition timing is a result of the error in the concentration profiles from setting species to steady state. Reactant species are of particular importance. In Fig. 4, the concentration profiles of OH and CO, respectively, are shown for mechanisms with an increasing degree of reduction. The profiles are obtained from the simulation described above at an inlet temperature of 1600 K. In all of the mechanisms, neither of the two species is set to steady state. The profiles are in good agreement with the detailed scheme for all but the most

reduced mechanisms, where some deviations are noticeable for both the CSP method and the lifetime analysis method. Less than 10% difference in mass fraction is found for mechanisms down to 15 steps. The ignition timing is better reproduced according to CSP. However, the maximum values are better modeled by the mechanism according to lifetime analysis. The differences in the mechanisms are that while the CSP model keeps HO_2 , OCHO, C_2H_2 , and $\text{C}_2\text{H}_5\text{OH}$ as major species, the lifetime analysis keeps H, C_2H_2 , C_2H_5 , and C_2H_3 as major species. The mechanism resulting from the lifetime analysis has at this point HO_2 in steady state. Since HO_2 is important for the ignition process, setting this species to steady state is thought to be responsible for the too early onset of the ignition. Even more reduced mechanisms give a significant error in the concentration profiles up to a deviation of 50% in maximum mass fraction.

When a similar validation procedure as illustrated in Fig. 2 is performed on the CSP-integrated pointers, the results look very similar. In Fig. 5, the same data as in Fig. 2 are compared with the corresponding integrated CSP pointers. The same main diagonal is found, thus revealing the consistency of the selection procedure. For both methods, some species lie off the main diagonal and will not be selected, although they are within the acceptable error limit for a given LOI or CSP pointer value. These species are found to be identical for the two methods with the exception of two species (OCHO and C_2H_2). The species lying off the diagonal are also found in the mechanisms as non-steady state (see Table 1). However, as discussed above, these species are assigned a larger error in LOI due to long lifetimes when compared with other steady-state species (see also Fig. 2). However, their sensitivities are low, leading to relatively less error being introduced to the system than for species with corresponding LOI.

Conclusions

A comparison between the steady-state species selected with CSP and those selected with a lifetime analysis based only on the diagonal elements of the Jacobian matrix and a species sensitivity was performed for a methane autoignition problem. Most of the steady-state species selected by the two methods were identical. The different species were related to fast timescales, which shows that for a large part of the timescale range, the diagonal estimate is reasonable. Both methods provided reduced mechanisms in good agreement with the detailed mechanism applied to an ignition process, as found by comparing mass fractions and ignition times. However, CSP seemed to achieve a given accuracy with mechanisms of smaller size. Nevertheless, the simpler and computationally faster lifetime analysis is of

sufficient accuracy and of greater convenience when applied to a system requiring a considerable reduction in computational time and for the chemical reduction procedure.

Acknowledgments

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COMMENTS

Marc Ribaucour, Université de Lille, France. Have you attempted to apply your automatic reduction procedures to detailed mechanisms developed to simulate the oxidation and autoignition of alkanes in the low temperature regime including the negative temperature region? If not, which level of reduction do you think it would be possible to achieve starting from a mechanism containing about 100 species and 1000 reactions with the goal to maintain the capacity of the reduced mechanism to reproduce the evolution of ignition delay time versus temperature and pressure?

Author's Reply. We have done work on reduced mechanisms for the low temperature regime, and the work is in progress. For alkanes it is possible to obtain reduced mechanisms of approximately 17–20 species from a set of originally 74 species reacting in 510 reactions [1]. The original mechanism is from Chevalier (C1–C4) and Muller (C5–C8). In this work, the mechanism was reduced to a skeletal mechanism by means of a reaction flow and sensitivity analysis to 63 species and 389 reactions. This mechanism was

the basis for further reduction by use of the LOI and the QSSA analysis, as described in the paper, to 19 species and 16 global reactions and still was able to reproduce the physical parameters with good accuracy. It should be noted that this work did not employ the adaptive scheme but the results should not differ. Since in the adaptive scheme the selection of the steady-state species are carried out locally, the low temperature phenomena are reproduced automatically. Please see Ref. [1] and further references therein.

Unpublished work suggests that the Westbrook mechanism containing 535 species and 4354 reactions can be reduced to a skeletal mechanism by use of reaction flow and sensitivity analysis to 250 species and 2144 reactions. Further reduction should bring the mechanism down to around 40 species.

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