Skeletal Mechanism Generation of Surrogate Jet Fuels for Aeropropulsion Modeling

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Abstract. A novel implementation for the skeletal reduction of large detailed reaction mechanisms using the directed relation graph with error propagation and sensitivity analysis (DRGEPSA) is developed and presented with skeletal reductions of two important hydrocarbon components, *n*-heptane and *n*-decane, relevant to surrogate jet fuel development. DRGEPSA integrates two previously developed methods, directed relation graph-aided sensitivity analysis (DRGASA) and directed relation graph with error propagation (DRGEP), by first applying DRGEP to efficiently remove many unimportant species prior to sensitivity analysis to further remove unimportant species, producing an optimally small skeletal mechanism for a given error limit. It is illustrated that the combination of the DRGEP and DRGASA methods allows the DRGEPSA approach to overcome the weaknesses of each previous method, specifically that DRGEP cannot identify all unimportant species and that DRGASA shields unimportant species from removal.

INTRODUCTION

Combustion of hydrocarbon fuels currently provides 85% of energy in the modern United States [1]. Renewable sources of energy are being pursued to supplement and eventually replace combustion-based sources, but hydrocarbons will remain the major component for the next few decades. In the current era of increasing environmental awareness and rising fuel costs, there is considerable demand to improve efficiency and reduce emissions of the next generation of combustion technology. Fuel-flexible designs that can use both conventional and alternative fuels are also desired.

Since computational modeling drives the design of engines and combustors for aerospace, transportation, and energy applications, accurate prediction of fuel combustion and pollutant emissions requires comprehensive detailed reactions mechanisms. However, detailed reaction mechanisms for surrogates of gasoline [2, 3], diesel [2, 4], and jet fuels [5, 6] typically contain large numbers of species and reactions. For instance, a recently developed detailed mechanism for *n*-alkane hydrocarbons C_8–C_{16} [7] contains 2115 species and 8157 reactions. Despite rapid advancements in computing power, it is generally formidable to integrate such detailed reaction mechanisms into large-scale computational simulations in terms of CPU time and memory requirements. In addition, the wide range of time scales (from nanosecond to second) and the nonlinear coupling between species and reactions induces stiffness when governing equations are solved [8]. Due to these computational demands, reduction of large mechanisms is necessary to facilitate practical simulations using detailed chemistry with modern computational tools.

Skeletal reduction is typically the first step of mechanism reduction, where species and reactions deemed negligible to important phenomena over the range of conditions of interest (e.g. pressure, temperature, and equivalence ratio) are removed from the detailed mechanism. Much effort has been dedicated to the development of effective skeletal reduction techniques, as reviewed by Tomlin et al. [9] and Okino and Mavrovouniotis [10].

The DRG approach has been shown to be a particularly efficient and reliable method to reduce large reaction mechanisms [11, 12]. The method uses a directed graph to map the coupling of species and consequently find unimportant species for removal, based on selected target species and an acceptable error threshold. Further development of the DRG method recently branched into two major directions: (1) DRG-aided sensitivity analysis (DRGASA) [13, 14], which performs sensitivity analysis not removed by DRG to further reduce the mechanism, and (2) DRG with error propagation (DRGEP) [15, 16], which considers the propagation of error due to species removal down reaction pathways. Another method based on DRG, path flux analysis [17], was recently presented that uses production and consumption fluxes to identify important reaction pathways. In the current work an approach that integrates the major aspects of DRGEP and DRGASA, DRG with error propagation and sensitivity analysis (DRGEPSA), is presented. It is illustrated that this combined approach overcomes the weaknesses of the two individual methods.

The current work is a continuation of previous demonstrations of the DRGEPSA method using a skeletal reduction of 1,3-butadiene [18] and initial skeletal reductions of *n*-heptane and *n*-decane [19]. In the following, the methodology of DRGEPSA for the skeletal reduction of large detailed reaction mechanisms is first discussed; in particular, components

important to surrogates of gasoline, diesel, and jet fuels are considered. The weaknesses of DRGEP and DRGEPSA, and the subsequent improvement of DRGEPSA, are demonstrated with a skeletal reduction of the *n*-heptane detailed mechanism of Curran et al. [20] A skeletal mechanism for *n*-decane from the mechanism of Westbrook et al. [7] covering wide ranges of conditions is then presented. A high-temperature skeletal mechanism for *n*-decane is also presented to illustrate the capability of the DRGEPSA method for reduction based on a specific set of conditions.

FIGURE 1. A directed relation graph showing path-dependent species coupling.

CONTENTS

Methodology

The reduction procedure begins with the use of SENKIN [21] in conjunction with CHEMKIN-III [22] to generate numerical solutions of constant volume autoignition using the detailed reaction mechanism over a range of initial conditions. The SENKIN time evolution results are used for the subsequent chemical kinetic analysis while the ignition delay times are used to assess the overall performance of the resulting skeletal mechanisms.

First, the DRGEP method is performed in an iterative manner using the SENKIN solutions from the detailed mechanism. The threshold used to identify and remove unimportant species is increased until the maximum error in ignition delay prediction for the given initial conditions reaches a user-specified limit; in this manner, the algorithm finds an optimally reduced skeletal mechanism with DRGEP. The remaining species are then divided into two groups: (1) "limbo" species for further sensitivity analysis and (2) important species for automatic retention. Sensitivity analysis is performed on the limbo species to further identify unimportant species, which are then removed until the global error reaches the user-specified limit. In all steps of the reduction process, reactions containing removed species are also eliminated from the mechanism. Specifics of each phase of the skeletal reduction are detailed as follows.

DRGEP Phase

The first phase of DRGEPSA is based on the DRGEP of Pepiot-Desjardins and Pitsch [16], which in turn is an extension of the original DRG of Lu and Law [11, 12, 23]. The current DRGEP implementation includes an improved definition of the direct interaction coefficients motivated by the shortcomings of the original definition [15] in situations with long chemical paths involving fast modes [11]. The current DRGEP approach uses a directed graph to map the coupling of species in a reaction system. The graph vertices represent species and directed edges between vertices represent species dependencies. The dependence of one species to another is based on a contribution to overall production rate; in other words, if one species needs another to accurately reproduce the overall production rate. This contribution is expressed with the direct interaction coefficient (DIC):

$$r_{AB} \equiv \frac{\left| \sum_{i=1,n_R} v_{A,i} \, \omega_i \, \delta_B^i \right|}{\max\left(P_A, C_A\right)}, \tag{1}$$

$$P_A = \sum_{i=1}^{n_R} \max\left(0, v_{A,i} \, \omega_i\right), \tag{2}$$

$$C_A = \sum_{i=1}^{n_R} \max\left(0, -v_{A,i} \, \omega_i\right), \tag{3}$$

$$\delta_B^i = \begin{cases} 1 & \text{if the } i\text{th elementary reaction involves species B,} \\ 0 & \text{otherwise,} \end{cases} \tag{4}$$

where A and B represent the species of interest (with dependency in the $A \rightarrow B$ direction) and i is the ith reaction. The DICs are calculated for all species at each data point from the SENKIN evolution data and the maximum values are used in the following analysis.

After mapping the system, a depth first search (DFS) is performing starting at user-selected target species (e.g. fuel, oxidizer, important radicals or pollutants) to find the dependency pathways for all species relative to the targets. A path-dependent interaction coefficient (PIC), $r_{AB,p}$, represents the error propagation down a certain pathway and is defined as the product of intermediate DICs between the target species A and species of interest B down a certain path p in the directed graph. An overall interaction coefficient (OIC), R_{AB}, is then defined as the maximum of all PICs between the targets and each species of interest. For example, Fig. 1 shows a simple reaction system where the overall dependence of species A on species D is expressed as:
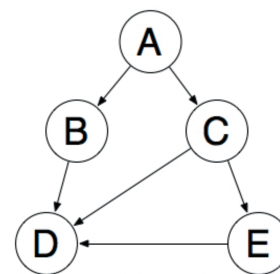
$$\text{DRG:} \quad R_{AD} = \max\left[\max\left(r_{AB}, r_{BD}\right), \max\left(r_{AC}, r_{CD}\right), \max\left(r_{AC}, r_{CE}, r_{ED}\right)\right]$$

$$\text{DRGEP:} \quad R_{AD} = \max\left[\left(r_{AB} \cdot r_{BD}\right), \left(r_{AC} \cdot r_{CD}\right), \left(r_{AC} \cdot r_{CE} \cdot r_{ED}\right)\right] ,$$

where path one is $A \rightarrow B \rightarrow D$, path two is $A \rightarrow C \rightarrow D$, and path three is $A \rightarrow C \rightarrow E \rightarrow D$.

The removal of species with OICs below a threshold ε_{EP} is considered negligible to the overall production rates of the target species and therefore such species are unimportant for the given conditions and can be removed from reaction system. The optimal threshold is chosen in an iterative manner in this DRGEP implementation. Using an initially low ε_{EP} (e.g. 0.01), a skeletal mechanism is generated and the error in ignition delay prediction is calculated for all initial conditions. If the maximum error for this skeletal mechanism is above the user-specified error limit, the threshold is decreased. For this and any subsequent mechanisms, if the maximum error is below the error limit the threshold is increased until the error reaches the specified limit. This procedure generates the minimum skeletal mechanism using DRGEP for a given error limit before sensitivity analysis is performed.

Sensitivity Analysis (SA) Phase

The second phase of DRGEPSA is based on the brute-force sensitivity analysis of Zheng et al. [13] In particular, species with OIC values above the final threshold ε_{EP} but below a higher value ε^* (e.g. 0.2–0.4) are classified as "limbo" species to be analyzed for removal. Species with OIC values greater than ε^* are classified as retained species and are automatically included in the final skeletal mechanism.

Limbo species are first removed from the mechanism one-by-one to find the resulting induced error in ignition delay then sorted in ascending order based on the absolute value of the difference between the induced error due to the removal of species B and the error of the DRGEP-generated mechanism. Many species do not change the mechanism error significantly compared to the DRGEP mechanism, so it is beneficial to remove the least important species first; using induced errors alone for species ranking would be incorrect. Species with an induced error above the specified error limit is removed from the list and retained in the final mechanism. The limbo species are then removed in order and the overall error is evaluated after each removal. The skeletal reduction is complete when the overall error reaches the user-specified error limit.

Results and Discussion

Skeletal Reduction of n-Heptane

n-Heptane is an important primary reference fuel (PRF) for gasoline with a zero octane number and is also important to diesel studies with cetane number similar to conventional diesel fuel [3, 4, 20]. Skeletal reductions of the detailed mechanism for n-heptane from Curran et al. [20], containing 561 species and 2539 reactions, were performed using DRGASA, DRGEP, and DRGEPSA to illustrate the individual weaknesses of the two original methods and the subsequent improvement of the combined method. All three methods used the same SENKIN evolution data; in addition, all methods used the iterative procedure described previously to determine the optimal error threshold value (ε_{EP} for DRGEP and DRGEPSA and ε_{DRG} for DRGASA). The ignition delay error limit was 30% for the iterative error threshold selection as well as the sensitivity analysis phases of DRGASA and DRGEPSA. Data was sampled from constant volume autoignition with initial conditions covering 600–1600 K, 1–20 atm, and equivalence ratio of 0.5–1.5. Oxygen, nitrogen, n-heptane, and the hydrogen radical were selected as target species for all reduction methods; the hydrogen radical was included to increase the extent of reduction for DRGEP and DRGEPSA for the given error limit. The DRG and DRGASA results were not affected by this inclusion because the DRG approach does not consider distance from targets in the directed graph and the hydrogen radical was already included in the dependent set.

The skeletal reduction results for n-heptane are shown in Table 1. Through the iterative threshold selection procedure, 0.16 was selected as the optimal ε_{DRG} to generate a mechanism of 211 species using DRG while 0.01 was selected as the
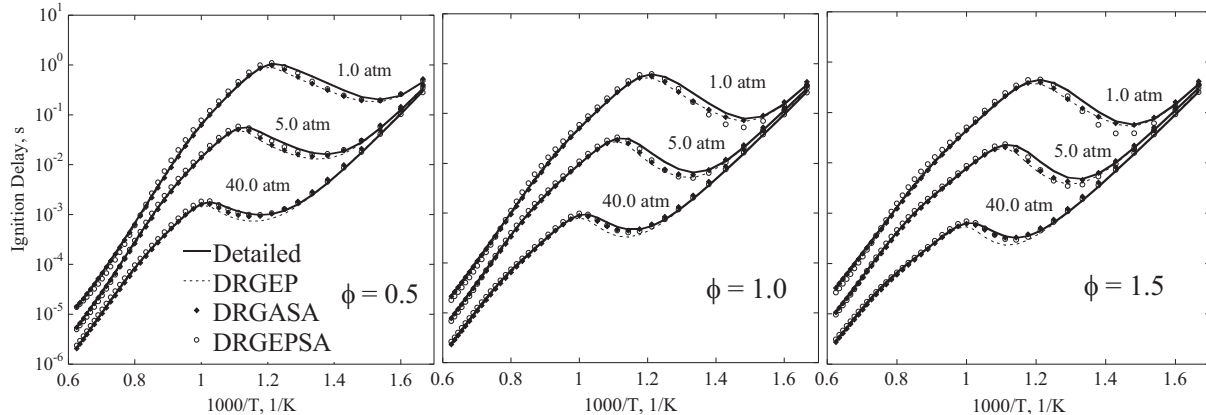
FIGURE 2. Autoignition validation of n-heptane skeletal mechanisms over a range of initial temperature, pressure, and equivalence ratio conditions.

optimal ε_{EP} to generate a mechanism of 173 species using DRGEP. It is seen that the DRGEP and DRGASA methods generate mechanisms of comparable size while DRGEPSA produces a smaller skeletal mechanism; all methods produce mechanisms of comparable performance.

Validation of the DRGEP, DRGASA, and DRGEPSA skeletal mechanisms was performed and is shown in Fig. 2, covering temperatures of 600–1600 K, pressures of 1, 5,

TABLE (1). Comparison of *n*-heptane skeletal mechanism sizes generated by DRG, DRGEP, DRGASA, and DRGEPSA.

Method	# Species	# Reactions	Max Error
DRG	211	1044	21%
DRGASA	153	691	24%
DRGEP	173	868	28%
DRGEPSA	108	406	27%

and 40 atm, and equivalence ratios of 0.5, 1.0, and 1.5. All three skeletal mechanisms exhibit good performance over the full range of conditions, but noticeable discrepancy (limited to 30% by the reduction procedure) occurs mainly in the negative temperature coefficient (NTC) region. It is interesting to note that at higher pressures, the larger DRGEP mechanism shows poorer performance in the NTC region than the smaller DRGASA and DRGEPSA mechanisms.

Figure 3 shows the species analyzed by sensitivity analysis (limbo species) in the DRGEPSA method. A highly nonlinear relationship is seen between the induced errors and the OIC values, illustrating the need for sensitivity analysis to further reduce the mechanism size. That is, simply increasing the ε_{EP} value would not be sufficient to remove unimportant species in this range of OIC values such that sensitivity analysis is needed following the DRGEP phase to generate a minimal skeletal mechanism. The OIC well represents the importance of lower-error species but may lose accuracy for species of higher importance and induced error.

The improvement of DRGEPSA over DRGASA is evident by the smaller final mechanism size and equivalent performance; DRGASA performs slightly better than DRGEP here, but the method cannot identify all unimportant species due to species "shielding." This occurs because the DRG phase uses a DIC to rank species [11, 12, 23], which does not consider distance from targets and can inflate species importance such that the species are automatically retained rather than considered with sensitivity analysis. Table 2 contains the results of the sensitivity analysis phase from DRGASA and DRGEPSA in the current comparison. 46 species out of the 129 species automatically retained by DRGASA; specifically, 17 were removed by the DRGEP phase and 29 were removed by the SA phase in DRGEPSA, illustrating the shielding effect in DRGASA. Species considered important enough to automatically retain by DRGASA are found unimportant and removed by DRGEPSA. Although this increases the extent of reduction, the greater number of species considered for sensitivity analysis can cause the DRGEPSA reduction to be more computationally expensive.

A skeletal mechanism for *n*-heptane was previously generated using the DRGASA method by Lu and Law [14], using a two-stage DRG followed by sensitivity analysis. This approach used a similar autoignition initial condition range but also included perfectly stirred reactor (PSR) and laminar flame speed kinetics data in the reduction procedure. In the first stage of DRG, using $\varepsilon_{DRG} = 0.1$ produced an initial mechanism with 290 species, while in the second stage, applying DRG again to the resulting mechanism, using $\varepsilon_{DRG} = 0.19$ produced a mechanism with 188 species and 939 reactions. Following the sensitivity analysis phase, a final skeletal mechanism with 78 species and 359 reactions was obtained with approximately 30% maximum error. While this reduction provided a skeletal mechanism smaller than both the DRGASA and DRGEPSA mechanisms shown here, the purpose of the current work was to compare the DRGEP, DRGASA, and DRGEPSA methods alone rather than specific strategies of employing such methods.

Skeletal Reduction of n-Decane

n-Decane is an important diesel surrogate component [4] and a primary component for jet fuel surrogates [5, 6]. Two skeletal mechanisms for *n*-decane were generated using the DRGEPSA method from the detailed mechanism for *n*-alkanes covering *n*-octane through *n*-hexadecane of Westbrook et al. [7] which contains 2115 species and 8157 reactions. The first skeletal reduction was performed using constant volume auto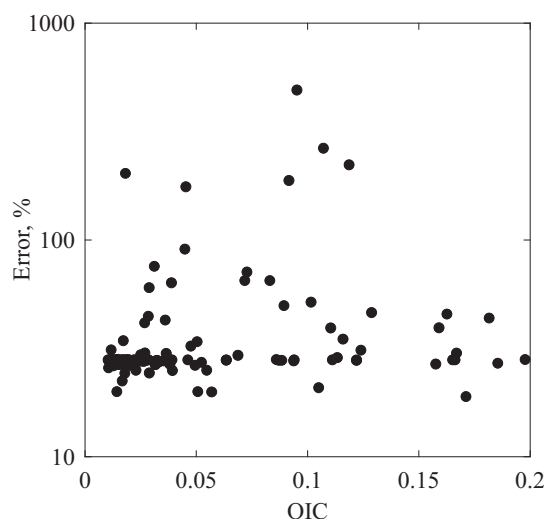ignition data sampled from initial conditions covering 600–1600 K and 1–20 atm, while the second skeletal reduction was limited to the high-temperature regime and atmospheric pressure, using 1000–1300 K, 1 atm; both covered equivalence ratios of 0.5–1.5. The error limit for both reductions was 30%; oxygen, nitrogen, *n*-decane, and the hydrogen radical were selected as target species for both reductions.

The DRGEP phase of the comprehensive reduction generated an initial skeletal mechanism with 381 species and 1865 reactions with a maximum error of 27% using $\varepsilon_{EP} = 1.4 \times 10^{-3}$. The final skeletal mechanism following sensitivity analysis contained 202 species and 846 reactions with a maximum error of 25%.

The DRGEP phase of the high-temperature reduction produced an initial skeletal mechanism with 68 species and

FIGURE 3. Induced error versus OIC values for species considered with sensitivity analysis phase in DRGEPSA.

TABLE (2). Comparison of DRGASA and DRGEPSA method sensitivity analysis results.

Method	# Retained	# Limbo	# Removed
DRGASA	129	82	58
DRGEPSA	54	119	65
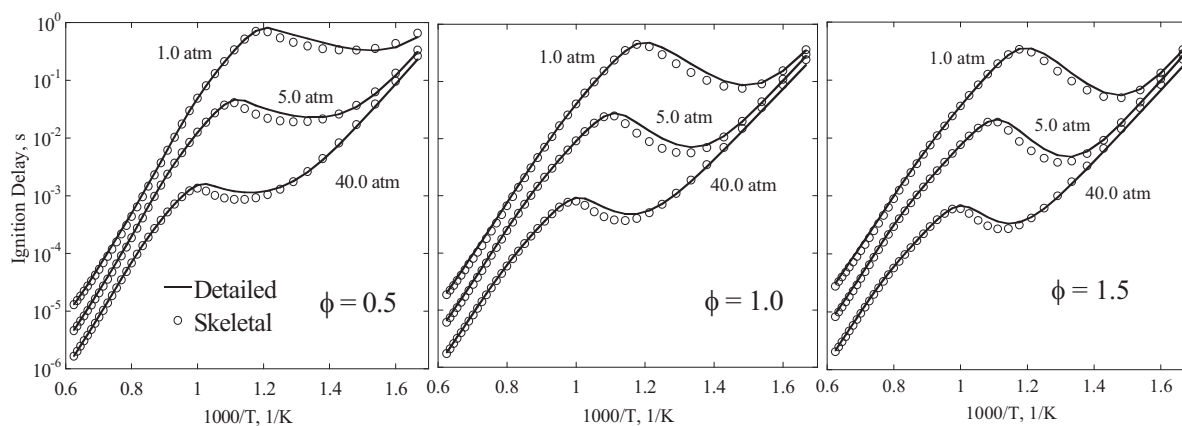
FIGURE 4. Autoignition validation of the *n*-decane comprehensive skeletal mechanism over a range of initial temperature, pressure, and equivalence ratio conditions.
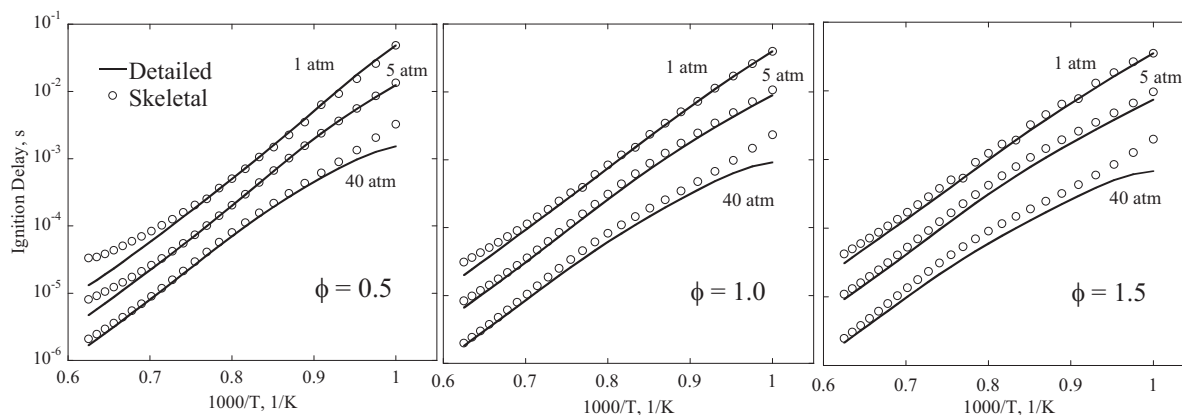
FIGURE 5. Autoignition validation of the *n*-decane high-temperature skeletal mechanism over a range of initial temperature, pressure, and equivalence ratio conditions.

391 reactions and a maximum error of 24%, using ε_{EP} = 0.007. Following sensitivity analysis, the final skeletal mechanism consisted of 45 species and 190 reactions with a maximum error of 27%.

Validation was performed using constant volume autoignition for both the comprehensive and high-temperature skeletal mechanisms, covering pressures of 1, 5, and 40 atm and equivalence ratios of 0.5–1.5 with temperatures of 600–1600 K and 1000–1600 K, shown in Fig. 4 and 5 respectively. The comprehensive mechanism well predicts the ignition delay compared to the detailed mechanism for the full range of validation conditions, with some discrepancy in the NTC region. The high-temperature mechanism also shows fairly good performance, with noticeable discrepancies primarily at the low-temperature, high-pressure region, as expected.

While a significant reduction is achieved with the comprehensive skeletal mechanism (approximately 10% of the detailed mechanism) using DRGEPSA, the final mechanism is still too large for full-scale simulations. Further reduction using techniques such as removal of unimportant reactions, isomer lumping, time-scale analysis (e.g. quasi-steady-state assumption) and diffusive species bundling [8, 14] is required before realistic computational simulations are feasible. However, the small size of the high-temperature skeletal mechanism illustrates the significant reduction ability when limiting the input conditions to a desired range; for instance, flame simulations rely largely on high-temperature chemistry such that a skeletal mechanism could omit the low-temperature and NTC regime chemistry with allowable error. The current high-temperature mechanism with 45 species and 190 reactions could be used without further reduction for large-scale simulations.

CONCLUSIONS

In the present work the directed relation graph with error propagation and sensitivity analysis (DRGEPSA) method for skeletal mechanism reduction was presented and discussed. This approach, a combination of the DRGEP and DRGASA methods, utilized the specific strengths of each individual method in order to diminish some of the weaknesses. DRGEP efficiently identifies and removes unimportant species while DRGASA utilizes sensitivity analysis to identify further unimportant species for removal at a greater computational expense. By combining the two, DRGEPSA is able to identify and remove more unimportant species than its precursors; however, the greater extent of reduction could come at a greater computational expense. A skeletal reduction of *n*-heptane was used to illustrate the improvement of DRGEPSA over DRGEP and DRGASA, generating a skeletal mechanism with 108 species compared to 173 and 153 species, respectively. All skeletal mechanisms exhibited good ignition delay prediction compared to the detailed mechanisms, with the most noticeable discrepancies in the NTC region.

Two skeletal reductions for *n*-decane from a large detailed mechanism for *n*-alkanes, covering *n*-octane through *n*-hexadecane, was additionally performed using DRGEPSA to illustrate the applicability of the method to the reduction of large mechanisms of surrogate fuels. One skeletal mechanism was generated to cover a comprehensive set of temperature conditions at moderately high pressures while the other was limited to high-temperature and atmospheric pressure conditions, and both mechanisms covered lean to rich equivalence ratios. The resulting comprehensive skeletal mechanism consisted of 202 species and 846 reactions while the high-temperature mechanism was much smaller with 45 species and 190 reactions.

The DRGEPSA method has been shown to remove large numbers of unimportant species and reactions more efficiently and with greater capabilities than previous DRG-based methods. Further reduction techniques would still needed in order to use the comprehensive skeletal mechanisms for the two hydrocarbon components presented, but the high-temperature skeletal mechanism for *n*-decane illustrates the capability of generating small condition-specific mechanisms.

ACKNOWLEDGMENTS

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