Optimisation of Reaction Mechanisms for Aviation Fuels Using a Multi-objective Genetic Algorithm

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Abstract. In this study a multi-objective genetic algorithm approach is developed for determining new reaction rate parameters for the combustion of kerosene/air mixtures. The multi-objective structure of the genetic algorithm employed allows for the incorporation of both perfectly stirred reactor and laminar premixed flame data into the inversion process, thus producing more efficient reaction mechanisms.

1 Introduction

Reduction of engine development costs, improved predictions of component life or the environmental impact of combustion processes, as well as the improved assessment of any industrial process making use of chemical kinetics, is only possible with an accurate chemical kinetics model. However, the lack of accurate combustion schemes for high-order hydrocarbon fuels (e.g. kerosene) precludes such techniques from being utilised in many important design processes. To facilitate further development, a procedure for optimising chemical kinetic schemes must be devised in which a reduced number of reaction steps are constructed from only the most sensitive reactions with tuned reaction rate coefficients. A novel method for automating the optimisation of reaction mechanisms of complex aviation fuels is developed in this paper.

Complex hydrocarbon fuels, such as kerosene, require more than 1000 reaction steps with over 200 species, see [1]. Hence, as all the reaction rate data is not well known, there is a high degree of uncertainty in the results obtained using these large detailed reaction mechanisms. A reduced reaction mechanism for kerosene combustion was developed in [2] and their mechanism is used in this paper to test the ability of GAs to retrieve the reaction rate coefficients.

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We note that various methods have been proposed in order to find a set of reaction rate parameters that gives the best fit to a given set of experimental data. However, in the case of complex hydrocarbon fuels, the objective function is usually highly structured, having multiple ridges and valleys and exhibiting multiple local optima. For objective functions with such a complex structure, traditional gradient based algorithms are likely to fail. Optimisation methods based upon linearization of the objective function, see [3] and [4], fall into the same category. On the other hand, genetic algorithms are particularly suitable for optimising objective functions with complex, highly structured landscapes.

A powerful inversion technique, based on a single objective genetic algorithm, was developed in [5] in order to determine the reaction rate parameters for the combustion of a hydrogen/air mixture in a perfectly stirred reactor (PSR). However, many practical combustors, such as internal combustion engines, rely on premixed flame propagation. Moreover, burner-stabilized laminar premixed flames are very often used to study chemical kinetics in a combustion environment. Such flames are effectively one-dimensional and can be made very steady, thus facilitating detailed experimental measurements of temperature and species profiles. Therefore, for laminar premixed flames it is much easier to obtain accurate experimental data to be used in the genetic algorithm inversion procedure. Therefore, in order to obtain a reaction mechanism which can be used for a wide range of practical problems it is required to use an inversion procedure which incorporates multiple objectives. Another reason to use this approach is the fact that sometimes in practical situations the amount of experimental data available is limited and it is important to use all the available experimental data, which may come from different measurements for perfectly stirred reactors or laminar premixed flames.

Therefore the single objective optimisation technique proposed in [5] is further extended to a multi objective genetic algorithm in order to include into the optimisation process data from premixed laminar flames. The algorithm was found to provide good results for small scale test problem, i.e. for the optimisation of reaction rate coefficients for a hydrogen/air mixture. It is the purpose of this paper to extend this technique to the case of complex hydrocarbon fuels.

An inversion procedure based on a reduced set of available measurements is also considered. In many experimental simulations, some of the species concentrations are subject to large experimental errors both in perfectly stirred rectors and laminar premixed flames. In order to facilitate the incorporation of various types of experimental data in the GA based inversion procedures, this study also investigates such GA calculations based on such incomplete or reduced sets of data.

2 Description of the Problem

2.1 Reaction Rate Parameters

In a combustion process the net chemical production or destruction rate of each species results from a competition between all the chemical reactions involving

that species. In this study it is assumed that each reaction proceeds according to the law of mass action and the forward rate coefficients are of three parameter functional Arrhenius form, namely

$$k_{f_i} = A_i T^{b_i} \exp\left(-\frac{E_{a_i}}{RT}\right) \tag{1}$$

for $i = 1, \ldots, N_R$, where R is the universal gas constant and there are N_R competing reactions occurring simultaneously. The rate equations (1) contains the three parameters A_i, b_i and E_{a_i} for the ith reaction. These parameters are of paramount importance in modelling the combustion processes since small changes in the reaction rates may produce large deviations in the output species concentrations. In both perfectly stirred reactors as well as in laminar premixed flames, if the physical parameters required are specified, and the reaction rates (1) are given for every reaction involved in the combustion process, then the species concentrations of the combustion products may be calculated. It is the possibility of the determination of these parameters for each reaction, based upon outlet species concentrations, which is investigated in this paper.

2.2 The Perfectly Stirred Reactor (PSR) Calculations and the Laminar Premixed Flames (PREMIX) Calculations

Various software packages may be used for the direct calculations to determine the output species concentrations if the reaction rates are known. In this study the perfectly stirred rector calculations are performed using the PSR FORTRAN computer program that predicts the steady-state temperature and composition of the species in a perfectly stirred reactor, see [6] while the laminar premixed flame structure calculations were performed using the PREMIX code, see [7].

We use X_k to denote the mole fraction of the kth species, where $k = 1, ..., K$ and K represents the total number of species. The temperature and composition which exit the reactor are assumed to be the same as those in the reactor since the mixing in the reactor chamber is intense.

If PSR calculations are undertaken for N_S^{PSR} different sets of reactor conditions then the output data which is used in the GA search procedure will consist of a set of mole concentrations, (X_{jk}, $j = 1, ..., N_S^{PSR}$, $k = 1, ..., K$), where X_{jk} represents the mole concentration of the kth species in the jth set of reactor conditions.

The laminar premixed flame structure calculations were performed using the PREMIX code for burner stabilised flames with a known mass flow rate. The code is capable of solving the energy equation in determining a temperature profile. However, throughout this investigation a fixed temperature profile was preferred and the reason for fixing the temperature was two fold. Firstly, in many flames there can be significant heat losses to the external environment, which are of unknown and questionable origin and thus troublesome to model. Secondly, the CPU time involved in arriving at the final solution was decreased significantly.

If all the physical operating conditions are specified then for a given set of reaction rates (1) the profiles of the species concentration and the burning velocity as functions of the distance from the burner's surface are calculated. If PREMIX calculations are performed for N_S^{PREMIX} different sets of operating conditions then the output data of the code which is used by the GA in the matching process consists of a set of species concentration profiles ($Y_{jk}(x)$, $j = 1, ..., N_S^{PREMIX}$, $k = 1, ..., K$) and a set of burning velocity profiles ($V_j(x)$, $j = 1, ..., N_S^{PREMIX}$), where Y_{jk} is the profile of the mole concentration along the burner for the kth species in the jth set of operating conditions and V_j is the burning velocity profile for the jth set of operating conditions.

It is the purpose of this paper to determine the reaction rate coefficients A's, b's and E_a's in equation (1) given species concentrations X_{jk} in a perfectly stirred reactor and/or profiles of species concentration Y_{jk} and the burning velocity profiles V_j in laminar premixed flames.

3 Reformulation of the Problem as an Optimisation Problem

An inverse solution procedure attempts, by calculating new reaction rate parameters that lie between predefined boundaries, to recover the profiles of the species (to within any preassigned experimental uncertainty) resulting from numerous sets of operating conditions. The inversion process aims to determine the unknown reaction rate parameters ((A_i, b_i,E_{a_i}), $i = 1, ..., N_R$) that provide the best fit to a set of given data. Thus, first a set of output concentration measurements of species is simulated (or measured). If numerical simulations are performed for N_S^{PSR} different sets of PSR operating conditions and/or N_S^{PREMIX} different sets of PREMIX operating conditions then the data will consist of a set of KN_S^{PSR} concentration measurements of species for PSR calculations and $(K + 1)N_S^{PREMIX}$ profiles of species concentrations and burning velocity for PREMIX calculations.

Genetic algorithms based inversion procedures seek for the set of reaction rate parameters that gives the best fit to these measurements. In order to do so we consider two objective functions which compare predicted and measured species concentrations for PSR and PREMIX simulations

$$f_{PSR}((A_i, b_i, E_{a_i})_{i=1,N_R}) = \left\{ 10^{-8} + \sum_{j=1}^{N_S} \sum_{k=1}^{K} W_k \frac{\left| X_{jk}^{calc} - X_{jk}^{orig} \right|}{X_{jk}^{orig}} \right\}^{-1} \tag{2}$$

$$f_{PREMIX}((A_i, b_i, E_{a_i})_{i=1,N_R}) = \left\{ 10^{-8} + \sum_{j=1}^{N_S} \left(\frac{\|V_j^{calc} - V_j^{orig}\|_{L^2}}{\|V_j^{orig}\|_{L^2}} + \sum_{k=1}^{K} W_k \frac{\left\|Y_{jk}^{calc} - Y_{jk}^{orig}\right\|_{L^2}}{\|Y_{jk}^{orig}\|_{L^2}} \right) \right\}^{-1} \tag{3}$$

where

- X_{jk}^{calc}, Y_{jk}^{calc} and V_j^{calc} represent the mole concentrations of the kth species in the jth set of operating conditions and the burning velocity in the jth set of

operating conditions using the set of reaction rate parameters $((A_i, b_i, E_{a_i})$, $i = 1, ..., N_R)$,
- X_{jk}^{orig}, Y_{jk}^{orig} and V_j^{orig} are the corresponding original values which were measured or simulated using the exact values of the reaction rate parameters,
- $\| \cdot \|_{L^2}$represents the L^2 norm of a function which is numerically calculated using a trapezoidal rule,
- W_k are different weights that can be applied to each species depending on the importance of the species.

It should be noted that the fitness function (2) is a measure of the accuracy of species concentrations predictions obtained by a given reaction mechanism for PSR simulations. The second fitness function (3) is a measure of the accuracy in predicting species concentrations and burning velocity profiles in the case of laminar premixed flames.

4 The Multi-objective Genetic Algorithm Inversion Technique

There is a vast variety of genetic algorithms approaches to multi-objective optimisation problems. GAs are in general a very efficient optimization technique for problems with multiple, often conflicting, object functions. However, most GA approaches require that all the object functions are evaluated for every individual generated during the optimisation process. For the problem considered in this paper, the object function f_{PREMIX} requires a long computational run time. For example, in the kerosene case a PREMIX run for one operating condition, $N_S^{PREMIX} = 1$, was found to take an average of 94 seconds CPU time on a Pentium IV processor running at 1.7GHz. This leads to a running time of more than 65 days, for evaluating say 1000 GA generations with 60 individuals generated at every iteration. On the other hand, PSR calculations are much faster, requiring for example an average of 14 seconds CPU time for evaluating one individual at $N_S^{PSR} = 18$ different operating conditions. Therefore, in this paper we propose a multi-objective GA that avoids PREMIX evaluations at every generation. The algorithm is based on alternating the fitness functions that are used for selecting the survivors of the populations generated during the GA procedure. Under the assumptions that the optimisation problem considered has n objective functions the multi-objective GA employed in this paper consists of the following steps

1. Construct n fitness functions $f_1, f_2, ..., f_n$ and assign a probability for each of these functions $p_1, p_2, ..., p_n$.
2. Construct an initial population.
3. Select a fitness function f_i with the probability p_i using a roulette wheel selection
4. Using the fitness function selected at step 3 construct a new population
   - Use the fitness function f_i to select a mating pool.

- Apply the genetic operators (crossover and mutation) to create population of offsprings.
- Use the fitness function f_i to construct a new population by merging the old population with the offsprings population.

5. Repeat steps 3-4 until a stopping condition is satisfied, i.e. convergence is achieved.

For the problem considered in this paper we have $n = 2$, $f_1 = f_{PSR}$, $f_2 = f_{PREMIX}$. Different values can be used for the fitness selection probabilities p_{PSR} and p_{PREMIX}. It is worth noting that the fitness selection probabilities p_{PSR} and p_{PREMIX} can be used to bias the convergence of the algorithm towards accurate predictions in PSR or PREMIX, respectively. However they do not act as weights since at every generation only one of the objective functions (2) and (3) is evaluated and not a linear combination of both of them. Instead these objective functions are alternated during the evolution process. This method maintains the multi-objective character of the optimisation process while avoiding the evaluation of the expensive fitness function (3) during every generation.

The CPU time required by the algorithm depends on the values set for the probabilities p_{PSR} and p_{PREMIX}. In this paper we have considered $p_{PSR} = 0.9$ and $p_{PREMIX} = 0.1$. For these values the genetic algorithm was found to require an average of 22 minutes/generation on a Pentium IV processor running at 1.7GHz. Numeircal experiments have been performed for various values for the selection probabilities p_{PSR} and p_{PREMIX} and it was found that the quality of the solution found in the end is not affected for a large range of values. However the CPU time can be controlled by choosing suitably these probabilities according to the number of PSR and PREMIx runs required.

We note that the GA employed is based on a floating point encoding of the variables. The genetic operators and the GA parameters were taken to be as follows: population size $n_{pop} = 50$, number of offspring $n_{child} = 60$, uniform arithmetic crossover, crossover probability $p_c = 0.65$, tournament selection, tournament size $k = 2$, tournament probability $p_t = 0.8$, non-uniform mutation, mutation probability $p_m = 0.5$, elitism parameter $n_e = 2$.

The new sets of rate constants generated every iteration are constrained to lie between predefined boundaries that represent the uncertainty associated with the experimental findings listed in the National Institute of Standards and Technology (NIST) database. The constraints are imposed by associating a very low fitness function to the individuals that violate these constraints.

It is worth noting that when working with accurate experimental data or numerically simulated data the two fitness functions (2) and (3) have a common global optimum given by the real values of the reaction rate coefficients or the values that were used to generate the data, respectively. Therefore for the problem considered the two objective functions are not conflicting and the method we have proposed can be used although it searches for a single common optima, rather than a set of non-dominated solutions. It is worth noting that if the experimental data is corrupted with a large level of noise then the two objective

functions (2) and (3) may be conflicting and then Pareto oriented techniques have to be used in order to construct the front of non-dominated solutions, i.e. a set of possible optima. In this situation other considerations have to be used to make a decision on what is the best location of the optimum.

5 Numerical Results

In order to test the multi-objective genetic algorithm inversion procedure, the test problem considered is the recovery of the species concentration profiles predicted by a previously validated kerosene/air reaction mechanism for a wide range of operating conditions which was presented in [2]. The reaction scheme used to generate the data involves $K = 63$ species across $N_R = 168$ reactions. Ideally, experimental data would have been preferred but at this developmental stage in order to avoid the uncertainty associated with experimental data it was decided to undertake numerical computations on a set of numerically simulated data. Since the purpose of this study is to develop and to assess the technical feasibility of the multi-objective GA techniques for the development of new reaction mechanisms for complex high order fuels in order to employ the most efficient schemes for future investigations concerning aviation fuels, for this study numerically simulated data is as efficient as experimental data.

The test problem considered is the combustion of a kerosene/air mixture at constant atmospheric pressures, $p = 10atm$ and $p = 40atm$. A set of $N_S^{PSR} = 18$ different operating conditions have been considered for PSR runs corresponding to various changes to the inlet temperature from *780K* to *1150K*. The inlet composition is defined by a specified fuel/air equivalence ratio, $\Phi = 1.0$ or $\Phi = 1.5$. Rather than solving the energy equation we assume that there is no heat loss from the reactor, i.e. $Q = 0$ and the temperature profile is specified.

For PREMIX calculations $N_S^{PREMIX} = 1$ for a steady state burner stabilized premixed laminar flames with specified temperature, pressure $p = 1atm$ and fuel/air equivalence ratio, $\Phi = 1.0$.

In many practical situations measurements are available only for the most important species. Therefore it is the purpose of this section to test the GA inversion procedure proposed also for the case of incomplete sets of data. Two reaction mechanisms are generated using two sets of data simulating complete and incomplete sets of measurements as follows:

- COMPLETE - is generated using multi-objective optimisation based on PSR and PREMIX data for all the output species
- REDUCED - is generated using multi-objective optimisation based on PSR and PREMIX data only for the following species: kerosene (C10H22+C6H5CH3), O2, C6H6, CO, CH2O, CO2, H2, C2H4, CH4, C3H6, C2H6, C2H2, C4H8

These two reaction mechanisms are used to produce estimations of the output species concentrations and these estimations are compared with the predictions given by the original mechanism (ORIGINAL), i.e. the mechanism which was used to simulate the data numerically, see [2].

5.1 Output Species Predictions for PSR and PREMIX Calculations

Figures 1 presents the unburned fuel concentration calculated with the PSR program, using the reaction mechanisms generated in the GA inversion procedure and the original mechanism for various temperatures and the air/fuel ratio given by $\Phi = 1.0$ at constant atmospheric pressures, $p = 10atm$. It can be seen that both the COMPLETE and REDUCED mechanism which were generated by the multi-objective GA are accurate in reproducing the output species concentrations as predicted by the original mechanism. Although not presented here, it is reported that also for the other species similar results were obtained. If the pro-

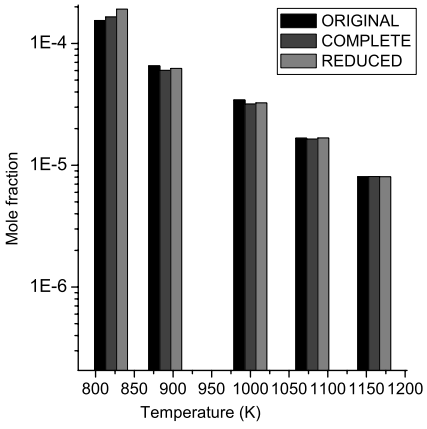

Fig. 1. The mole fraction of unburned fuel for various temperatures and air/fuel ratio given by $\Phi = 1.0$ at constant atmospheric pressures, $p = 10atm$ as predicted by various reaction mechanisms in PSR calculations.

files of the mole fractions in the PREMIX calculations are investigated, then the GA generated reaction mechanisms are again found to be efficient in predicting the species profiles, see Figure 2 which presents the output species profiles of four major species for a pressure p = 1atm and fuel/air equivalence ratio, $\Phi = 1.0$. It can be seen that both mechanisms generated by our inversion procedure are efficient in predicting the mole fractions even for very low concentrations. Many other species have been investigated for PSR and PREMIX calculations for operating conditions within the range used for the optimisation process and overall it was found that the reaction mechanisms generated by the GA are accurately reconstructing the output species predicted by the original mechanism.

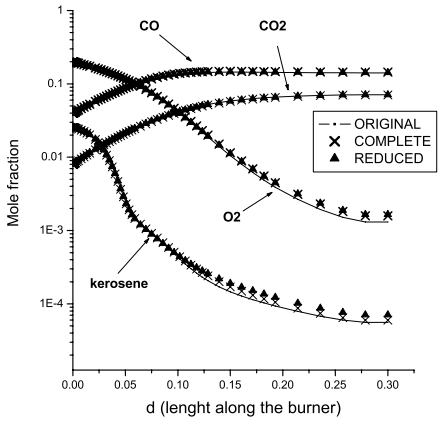

Fig. 2. The species profiles of various output species for premixed laminar flames as predicted by various reaction mechanisms, namely the original mechanism (-), the COMPLETE mechanism (×) and the REDUCED mechanism (▲).

5.2 Validation of the GA Generated Mechanisms for Various Operating Conditions

The previous section presented the predictions given by the constructed reaction mechanisms for operating conditions which were included in the optimisation process. However, the aim of the inversion procedure is to develop reaction mechanisms that are valid over wide ranges of operating conditions. Therefore, next the GA generated reaction mechanisms were tested at operating conditions outside the range included in the optimisation procedure. Figure 3 presents the species concentrations obtained by PSR calculations for the two GA generated reaction mechanisms, in comparison with those generated by the original mechanism for kerosene concentration at temperatures outside the range used for optimisation, i.e. $T = 1000K - 2000K$. Again it can be seen that the mechanisms COMPLETE and REDUCED give accurate predictions in comparison with the original mechanism. Figure 4 presents the predicted concentrations profiles of four of the main species obtained by PREMIX calculations at a constant atmospheric pressure $p = 2atm$ which is outside the range of operating conditions used for optimisation. It is worth noting that both COMPLETE and REDUCED reaction mechanisms are able to accurately predict the species concentration profiles for PREMIX operating conditions outside the range used for optimisation. It is worth noting that for some species, see Figure 4 it was found that the REDUCED mechanism is more efficient than the COMPLETE mechanism in particular in the part of the species profiles where the concentration is becoming very low. This can be explained by the fact that the REDUCED mechanism is biased towards some of the species and it predicts them very accurately while the COMPLETE mechanism is forced to predict with reasonable accu-

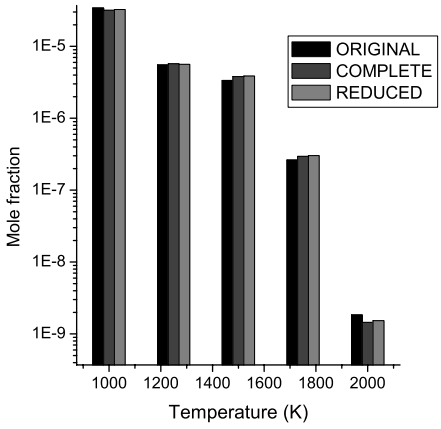

Fig. 3. The mole fraction of unburned fuel for various temperatures *T=1000K-2000K* as predicted by various reaction mechanisms in PSR calculations.

racy all the species, which is undertaken at the expense of slightly less accurate predictions for the main species. The REDUCED mechanism outperformed the COMPLETE mechanism only for those species which were included in the REDUCED inversion procedure while the COMPLETE mechanism outperformed the REDUCED mechanism if all the species are taken into consideration. It is worth mentioning that when working with numerically simulated data both mechanisms can be generated but in practice, it is impossible to obtain measurements for all the output species and therefore a reaction mechanism of the type REDUCED is generated when working with experimental data. Similar conclusions have been obtained for a wide range of operating conditions. Overall, the reaction mechanisms generated by the multi-objective GA proposed in this study were found to be very efficient in predicting the output species concentrations and burning velocity for both PSR and PREMIX simulations. Thus we may conclude that the inversion procedure proposed efficiently generates a general reaction mechanism that can be used to predict the combustion products for various combustion problems at a variety of operating conditions.

5.3 Ignition Delay Time Validations

To provide additional validation of the results obtained by the inversion procedures presented in this paper, the predicted ignition delay times are computed using all the reaction mechanisms generated in this study. In testing the ignition delay time, the SENKIN code of Sandia National Laboratories [8] was used to predict the time dependent chemical kinetic behaviour of a homogeneous gas mixture in a closed system.

Figure 5 compares the ignition delay times predicted by the reaction mechanisms generated in this study with the ignition delay times generated by the

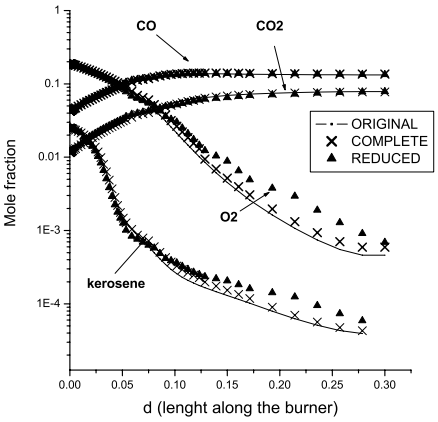

Fig. 4. The species profiles of various output species for premixed laminar flames at pressure $p = 2atm$ and fuel/air equivalence ratio, $\Phi = 1.0$ as predicted by various reaction mechanisms, namely the original mechanism (-), the COMPLETE mechanism ($\times$) and the REDUCED mechanism (▲).

original mechanism at four different initial temperatures and the air/fuel ratio $\Phi = 1.0$. We note that both the COMPLETE and the REDUCED mechanisms based on complete or incomplete sets of data, respectively, reproduce the same ignition delay times as the original mechanism and this indicates that the GA does not just generate a mechanism whose validity only extends as far as those operating conditions included in the optimisation process.

6 Conclusions

In this study we have developed a multi-objective GA inversion procedure that can be used to generate new reaction rate coefficients that successfully predict the profiles of the species produced by a previously validated kerosene/air reaction scheme. The new reaction rate coefficients generated by GAs were found to successfully match mole fraction values in PSR simulations and burning velocity and species profiles in PREMIX simulations, as well as ignition delay time predicted by the original starting mechanism over a wide range of operating conditions, despite their origin being based solely on measurements for a restricted range of operating conditions.

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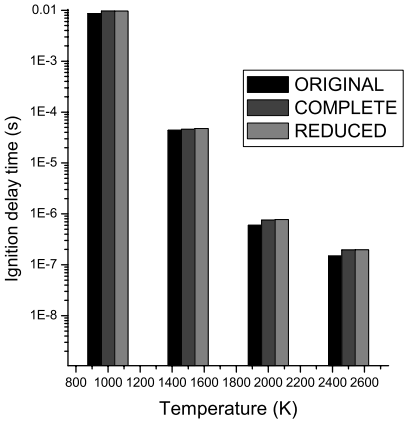

Fig. 5. The ignition delay time at various temperatures T=1000K-2500K as predicted by various reaction mechanisms.

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