An Informed Operator Based Genetic Algorithm for Tuning the Reaction Rate Parameters of Chemical Kinetics Mechanisms

Lionel Elliott[1], Derek B. Ingham[1], Adrian G. Kyne[2], Nicolae S. Mera[2], Mohamed Pourkashanian[2], and Christopher W. Wilson[3]

[1] Department of Applied Mathematics, University of Leeds, Leeds, LS2 9JT, UK, {lionel,amt6dbi}@amsta.leeds.ac.uk

[2] Centre for Computational Fluid Dynamics, Energy and Resources Research Institute, University of Leeds, Leeds, LS2 9JT, UK, {fueagk,fuensm,fue6lib}@sun.leeds.ac.uk

[3] Department of Mechanical Engineering, Mappin Street, University of Sheffield, Sheffield, S1 3JD, UK, c.w.wilson@sheffield.ac.uk

Abstract. A reduced model technique based on a reduced number of numerical simulations at a subset of operating conditions for a perfectly stirred reactor is developed in order to increase the rate of convergence of a genetic algorithm (GA) used for determining new reaction rate parameters of chemical kinetics mechanisms. The genetic algorithm employed uses perfectly stirred reactor, laminar premixed flame and ignition delay time data in the inversion process in order to produce efficient reaction mechanisms that are valid for a wide range of combustion processes and various operating conditions.

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. The process of optimising the reaction rates for complex hydrocarbon fuels is a computationally intensive procedure. Therefore it is required to devise fast methods for tuning the reaction rate parameters of various types of fuels.

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 linearisation of the objective function fall in the same category, see

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[1]. 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 genetic algorithm, was developed in [2] in order to determine the reaction rate parameters for the combustion of a kerosene/air mixture in a perfectly stirred reactor (PSR) and in premixed laminar flames (PREMIX). In order to obtain a reaction mechanism which can be used for a wide range of practical problems we also extend the work of [2] to include data from ignition delay time measurements. It is important to use this approach since in many 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 various types of measurements. Ignition delay times are easier to measure experimentally and therefore there is a larger amount of experimental data available for various fuels.

A real coded genetic algorithm, is employed in this paper since it was found that algorithms of this type accurately model the continuous search space of numerical optimisation problems. The rate of convergence of the genetic algorithm employed is accelerated by using a reduced model implemented within the frame of the informed operators technique proposed in [3]. However, rather than using polynomial approximations, neural networks or Kriging models to build the reduced model for the informed operators, in this paper we use a reduced number of PSR numerical simulations at a subset of operating conditions to provide useful information about the fitness function landscape to the informed operators. The method used in our study is a variation of the injection island genetic algorithm (iiGA), see [4], used for problems involving finite element analysis models.

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 those 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 i^{th} reaction. These parameters are of paramount importance in modeling the combustion processes since small changes in the reaction rates may produce large deviations in the output species concentrations. It is the possibility of the fast and efficient determination of these parameters for each reaction, based upon outlet species concentrations and ignition delay times, which is investigated in this paper.

2.2 The Perfectly Stirred Reactor (PSR) Calculations, the Laminar Premixed Flames (PREMIX) Calculations and the Ignition Delay Time (SENKIN) 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 computer program that predicts the steady-state temperature and composition of the species in a perfectly stirred reactor, see [5], while the laminar premixed flame structure calculations were performed using the PREMIX code, see [6] and the ignition delay time calculations are performed using the SENKIN code, see [7].

If PSR calculations are undertaken for N_S^{PSR} 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 k^{th} species in the j^{th} set of reactor conditions.

The laminar premixed flame structure calculations were performed using the PREMIX code for burner stabilized flames with a known mass flow rate. 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 k^{th} species in the j^{th} set of operating conditions and V_j is the burning velocity profile for the j^{th} set of operating conditions.

In calculating the ignition delay times, the SENKIN code of Sandia National Laboratories [7] was used to predict the time dependent chemical kinetic behaviour of a homogeneous gas mixture in a closed system. If all the physical operating conditions are specified then for a given set of reaction rates (1) the ignition delay times t_j, $j = 1, ..., N_S^{SENKIN}$ are calculated together with the first-order sensitivity coefficients.

2.3 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.

The GA inversion procedure proposed seeks for the set of reaction rate parameters that gives the best fit to these measurements. In order to do so we consider three objective functions which compare predicted and measured species concentrations, burning velocities and ignition delay times:

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

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

$$f_{SENKIN}((A_i, b_i, E_{a_i})_{i=1,N_R}) = \left\{ 10^{-3} + \sum_{j=1}^{N_S} \frac{\left| t_j^{calc} - t_j^{orig} \right|}{t_j^{orig}} \right\}^{-1} \quad (4)$$

where

- X_{jk}^{calc}, Y_{jk}^{calc} and V_j^{calc} represent the mole concentrations of the k^{th} species in the j^{th} set of operating conditions and the burning velocity in the j^{th} 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.
- t_j^{calc} and t_j^{orig} represent the calculated and the measured or simulated ignition delay times in the j^{th} set of operating conditions.

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 while the last fitness function (4) is a measure of the accuracy in predicting ignition delay times.

3 The Genetic Algorithm Optimisation Technique

3.1 A Standard Real Coded Genetic Algorithm

In this study we use a constrained genetic algorithm similar to the one proposed in [2]. The genetic operators and the parameters used for this genetic algorithm were taken to be population size $n_{pop} = 20$, number of offspring $n_{child} = 30$, non-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 $p_m = 0.5$.

It is worth noting that when working with accurate experimental data, or numerically simulated data, the three fitness functions (2), (3) and (4) 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 the three objective functions are not conflicting and we can optimise them simultaneously using a product objective function of the form:

$$f = f_{PSR} \cdot f_{PREMIX} \cdot f_{SENKIN} \quad (5)$$

although it searches for a single common optima rather than a set of non-dominated solutions. If the experimental data is corrupted with a large level of noise then the three objective functions (2), (3) and (4) 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.

3.2 Informed Operators Using a Subset of Operating Conditions

It is the purpose of this section to present an informed operators based genetic algorithm (IOGA) that uses a reduced subset of PSR or SENKIN operating conditions for guiding the GA search. In some optimisation tasks, the functions to optimise are analytical expressions that take a negligible amount of time to compute. However, in the case of realistic engineering design problems the optimisation function is a computationally expensive code which can take up to several hours of CPU time. Consequently it is desirable to use reduced models which are usually much faster than the actual objective function. Reduced models can be mathematical approximations, such as response surface induced using some evaluations of the original expensive model, can be simpler models relying on simpler equations like one-dimensional approximations, etc., or can be approximations based on a different level of discretisation, such as the injection island model.

Often the reaction rates retrieval problem described in section 2 requires a large number of operating conditions to be considered in the optimisation process in order to generate a widely applicable reaction mechanism. This leads to large computational times spent in evaluating one possible solution for the reaction rates. Often within the GA search these expensive evaluations are performed for an individual which is far from being an acceptable solution, and in this way much computational time is wasted on evaluations which do not provide any further information on the solution of the problem. In particular, PREMIX evaluations require a large CPU time. For complex hydrocarbon fuels the CPU time can build up to several months even if only one PREMIX operating condition is used, see [2].

In order to avoid expensive PREMIX evaluations for reaction mechanisms that are far from being an accurate solution, it is the purpose of this paper to implement a reduced model based on a subset of PSR or SENKIN operating conditions in order to pre-evaluate the GA generated solutions, and then to decide which individuals should be evaluated with the original expensive model. Thus, if the problem considered requires the evaluation of the reaction mechanism at N_S^{PREMIX} PREMIX operating conditions, N_S^{PSR} PSR operating conditions and N_S^{SENKIN} SENKIN operating conditions to obtain accurate approximations, the idea of reduced models is based on extracting information from evaluations at only $N'_{PSR} < N_S^{PSR}$ PSR operating conditions, information which is used to guide the search and to decide which solutions are evaluated with the full fitness function (5). The reduced model is implemented within the frame of informed

operators technique, see [3]. This approach has the advantage that it does not require assumptions about the accuracy of the reduced model. The assumption that computations at a subset of PSR operating conditions can accurately predict computations for a wider range of operating conditions, for PSR, PREMIX and SENKIN, does not hold in many practical problems. However in the informed operators approach the only requirement is that the reduced model is a better than random approximation of the accurate one. This approach is also simple and easy to implement into a genetic algorithm. The only difference between GA described in section 3, which will be referred to as the "standard GA" and the informed operators based GA (IOGA) is the replacements of the mutation and crossover operators with the following operators:

- **Informed mutation** To do mutation several random mutations are generated of the base point. Each mutation is generated by randomly selecting the parameters for the original mutation method. The off-springs created are evaluated using the reduced model based on N'_{PSR} PSR operating conditions. The mutation that appears best according to the reduced model is returned as the result of the mutation operator.
- **Informed crossover** To do crossover two parents are selected at random according to the original selection strategy. These two parents will not change in the course of the informed crossover operation. Several crossover are conducted by randomly selecting the internal parameters of the crossover operator. Each individual generated is evaluated with the reduced model and the best is considered to be the outcome of the crossover operator.

The number k of random mutations and crossovers applied for generating mutated or recombined children is an internal parameter of the IOGA and various values are investigated in this paper.

It should be noted that the informed operator technique employed in this study resembles the local search memetic algorithms discussed in [8]. However, such real coded memetic algorithms require many evaluation of the full fitness function to perform the local search and this is not feasible for computationally expensive problems such as the one illustrated here. Instead, in this study we employ in the search process a reduced model that incorporates problem specific knowledge. Other reduced models using response surfaces constructed from polynomial approximations, neural networks, Kriging models or support vector machines can be employed and they are very efficient for problems with reduced numbers of parameters, see [3]. However, for the problem of retrieving reaction rate coefficients, the number of unknown parameters is very large. For the combustion of hydrogen/air mixture there are 57 parameters to be identified, for $N_R = 19$ reactions, but for complex aviation fuels the number of unknown parameters can exceed 1000, which prohibits the application of such reduced models. However, the reduced model using subsets of operating conditions as described in this study can be applied also for complex reaction mechanisms with large numbers of reactions. Moreover, other response surface models which do not incorporate problem specific knowledge may lead the algorithms toward false optima. The reduced model employed in this study extracts information

from a reduced set of operating conditions, thus enabling a higher degree of confidence in its predictive capabilities.

4 Numerical Results

In order to test the informed operators based genetic algorithm inversion procedure the test problem considered is the recovery of the species concentration profiles predicted by a previously validated hydrogen/air reaction mechanism for a wide range of operating conditions. The reaction scheme used to generate the data involves $K = 9$ species across $N_R = 19$ reactions.

The test problem considered is the combustion of a hydrogen/air mixture at constant atmospheric pressures, $p = 1\,atm$ and $p = 10\,atm$. A set of $N_S^{PSR} = 10$, $N_S^{PREMIX} = 10$ and $N_S^{SENKIN} = 10$ different operating PSR, PREMIX and SENKIN operating conditions have been considered corresponding to various changes to the temperature from $1000K$ to $2000K$. The inlet composition is defined by a specified fuel/air equivalence ratio, $\Phi = 1.0$.

Several different mechanisms are generated using a GA optimisation process as follows

- **STANDARD** is a chemical reaction mechanism obtained by optimising the fitness function (5) by the standard GA described in section 3 without using informed operators.
- **IOGA-PSR** is a chemical reaction mechanism obtained by optimising the fitness function (5) by the IOGA described in section 3.2 using informed operators based on a subset of $N'_{PSR} = 4$ PSR operating condition evaluations.
- **IOGA-SENKIN** is a chemical reaction mechanism obtained by optimising the fitness function (5) by the IOGA described in section 3.2 using informed operators based on a subset of $N'_{SENKIN} = 4$ SENKIN operating conditions evaluations.

The operating conditions used for the informed operators are taken to be the bounds of the range used as operating conditions in the full optimisation process, i.e. $p = 1\,atm$ and $p = 10\,atm$ and $T = 1000K$ and $T = 2000K$. The GA generated 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.

Figure 1 presents the fitness functions obtained by the IOGA using PSR or SENKIN information with $k = 3$ in comparison with the fitness function obtained by the standard GA. It should be mentioned that all the results presented in this paper are obtained as the average of five different GA runs for five different sequences of random numbers. The graphs have been scaled such that they represent the results obtained in similar CPU times. The time unit that appears of the x-axis of Figure 1 is equivalent to the CPU time required to perform one whole generation in the standard GA and and is approximately 318 seconds of CPU time.

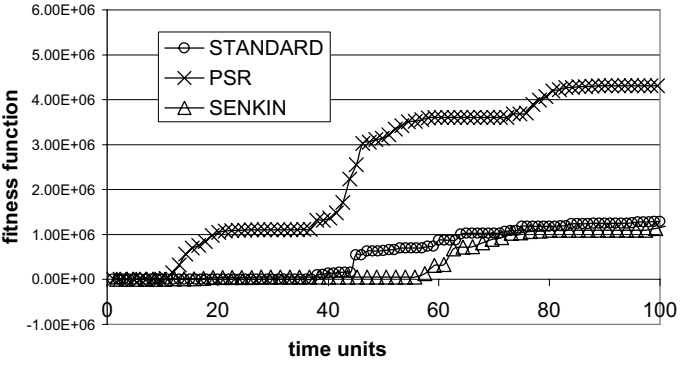

Fig. 1. The fitness functions for the standard GA and the informed operators based GA using perfectly stirred reactor evaluations (PSR) and ignition delay time evaluations (SENKIN).

It can be seen in Figure 1 that the IOGA-PSR clearly outperforms the standard GA. The PSR informed GA reaches the maximum value attained by the standard GA in about 1/5 of the CPU time required in the standard GA. However, the informed GA using SENKIN operating conditions is performing even worse than the standard GA. This can be explained by the fact that the SENKIN simulations only provide information about ignition delay times, while both PSR and SENKIN use information about the species concentration. The SENKIN object function (4) has multiple global optima since there are several sets of parameters that give exact predictions of ignition delay times but not all of these sets are accurate in predicting the species concentration. If a GA is employed to optimise only the SENKIN fitness function (4) then the reaction mechanism generated, GA-SENK, is very accurate in predicting the ignition delay time but is poor in predicting species concentrations. Figure 2 presents the O mole fractions in a PSR predicted by the GA-SENK mechanism in comparison with the original mechanism and the GA-ALL mechanism obtained by optimising the global fitness function (5) for PSR, PREMIX and SENKIN. It can be seen that if a mechanism is only optimised for SENKIN then it does not produce good results for PSR and PREMIX. However, mechanisms optimised for PSR and/or PREMIX, produce reasonably accurate results for SENKIN simulations as well, see [2]. Similarly, if an objective function based only on SENKIN evaluations is used in the informed operators then the search is possibly guided toward some false optima which correspond to reaction mechanisms efficient for ignition delay time predictions but not for species concentrations. This explains why the IOGA-PSR clearly outperforms the standard GA while the SENKIN informed operators do not improve the convergence rate of the GA. Therefore we will focus in the remainder of this study on PSR informed operators.

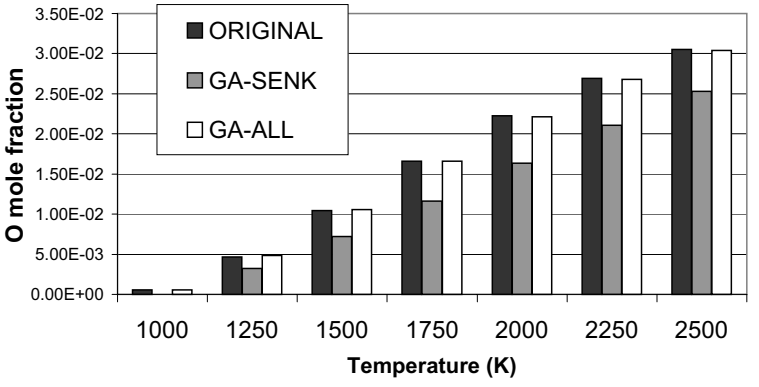

Fig. 2. The mole fraction of O in a perfectly stirred reactor at pressure $p = 1\,atm$ and air fuel ration $\Phi = 1.0$ for various temperatures as predicted by reaction mechanisms obtained by GA optimisations against ignitions delay time measurements (GA-SENK), or against ignition delay time measurements and species concentrations (GA-ALL) compared with the mole fractions predicted by the original mechanism.

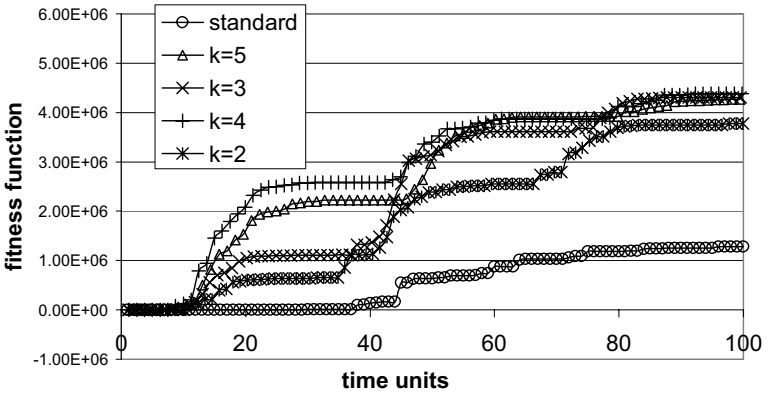

Fig. 3. The fitness functions for standard GA and the informed operators based GA using various numbers of mutations and crossovers, k, for informed operators based on $N'_{PSR} = 4$ PSR evaluations.

Figure 3 presents the evolution of the fitness function (5) values for the IOGA-PSR algorithm for various values of k, the number of trial mutations and crossovers that are generated and evaluated using the reduced model. It can be seen for all the values of k, IOGA outperforms the standard GA, reducing the CPU time required to obtain the same maximum value by a factor of up to 5. Similar results are obtained for larger values of k, see Figure 4 which presents the corresponding fitness functions for $k \in \{10, 15, 20\}$. Various values of the

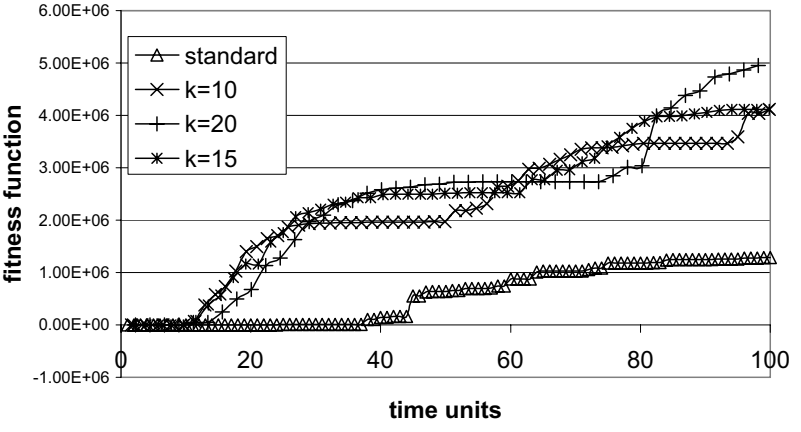

Fig. 4. The fitness functions for the informed operators based GA using large numbers of mutations and crossovers, $k \in \{10, 15, 20\}$, for informed operators based on $N'_{PSR} = 4$ PSR evaluations, in comparison with the fitness obtained for the standard GA.

parameter k have been investigated and the best results were observed if the time spent in evaluations using the fitness function (5) is balanced with the time spent in reduced model evaluation, i.e. if k is chosen such that within a GA generation, the time spent on reduced model evaluations is from one to four times the CPU time spent on evaluations with the fitness function (5).

4.1 Validation of the IOGA Generated Mechanisms for Various Combustion Processes

It is the purpose of this section to validate the mechanisms generated by the IOGA by comparing their predictions for PSR, PREMIX and SENKIN simulations with those obtained by the original mechanism. Figure 5 presents the O mole fractions obtained in PSR simulations as predicted by the original mechanism and the two mechanisms generated by the standard GA and the IOGA-PSR for $k = 5$, for various operating conditions, namely pressure $p = 1\,atm$, air fuel ration $\Phi = 1.0$ and various temperatures $T = 1000K, ..., 2000K$. It can be seen that similar species concentrations are predicted by all three mechanisms. 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. Figure 6 compares the ignition delay times predicted by the reaction mechanisms generated in this study with the ignition delay times generated by the original mechanism. We note that both the the standard GA and the IOGA produced mechanisms reproduce the same ignition delay times as the original mechanism. Although not presented here it is reported that the GA generated mechanisms produce accurate results also for PREMIX numerical simulations. The IOGA generated mechanism was tested at various other operating conditions and it was found to produce accurate pre-

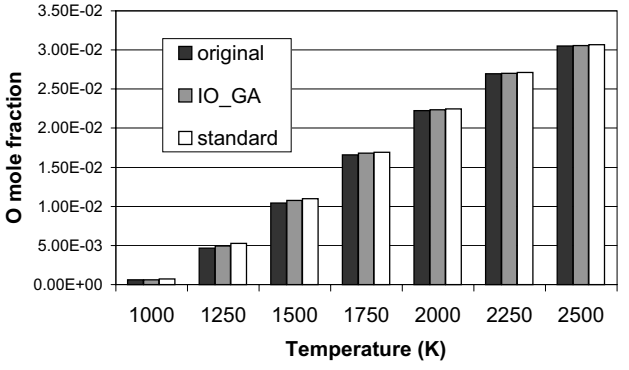

Fig. 5. The mole fraction of O in a perfectly stirred reactor at pressure $p = 1\,atm$ and air fuel ration $\Phi = 1.0$ for various temperatures as predicted by reaction mechanisms obtained by the standard GA and the informed operators based GA, compared with the mole fractions predicted by the original mechanism.

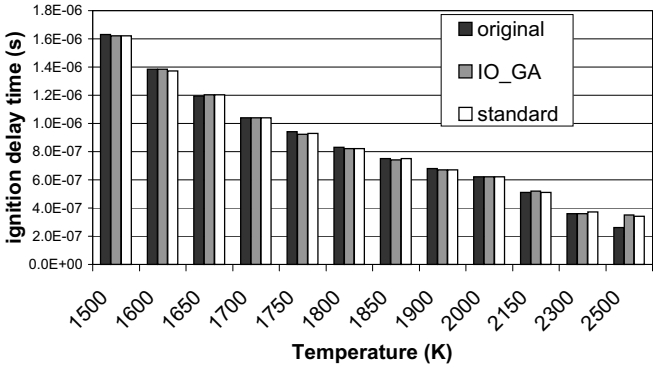

Fig. 6. The ignition delay times at pressure $p = 10\,atm$ and air fuel ration $\Phi = 1.0$ for various temperatures $T \in \{1500, ..., 2500\}$ as predicted by reaction mechanisms obtained by the standard GA and the informed operators based GA, compared with the mole fractions predicted by the original mechanism.

dictions for a wide range of operating conditions and various type of numerical simulations of combustion processes.

5 Conclusions

In this paper the problem of retrieving reaction rate coefficients for the combustion hydrogen/air mixtures under various operating conditions has been investi-

gated using a reduced model based GA. Informed GA operators using a subset of PSR simulations were used to speed-up the optimisation process. The reaction mechanism developed was tested for several test examples. The new reaction rate coefficients generated by the IOGA 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.

It was found that informed operators technique using subsets of PSR simulations is very efficient in guiding the GA operators toward more promising regions of the search space. The numerical results presented have shown that the computational time required to achieve an efficient reaction mechanism in the GA can be reduced up to five times by employing the informed operators technique.

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