

Optimization of Rate Coefficients for Global Reaction Mechanisms using a Nested Genetic Algorithm

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Abstract

In this paper a method is presented which optimizes the Arrhenius rate coefficients of global 2- and 3-step reaction mechanisms by fitting ignition delay time (τ_{ign}) and temperature profile for lean premixed methane combustion at high temperatures against data obtained from a detailed mechanism. While various global mechanisms are available to predict laminar flame speeds, their ability to predict τ_{ign} for high temperature combustion is limited. A nested genetic algorithm (GA) is used as optimization tool since traditional gradient based algorithms are likely to fail when highly complex fitness functions are regarded. Results are shown for both 2- and 3-step global reaction mechanisms and the applicability of the derived mechanisms on off-design conditions is discussed.

Introduction

In recent years continuous advancements in the numerical modeling of turbulent reacting flows could be achieved due to the development of better physical models, extensive investigation of detailed combustion models, improved computer hardware and better numerical algorithms. In order to describe combustion processes in applications of technical interest, though, the combined simulation of turbulent flow together with detailed combustion chemistry is still out of reach due to excessive computational cost. Therefore reduced chemistry models have been developed which are capable of describing combustion processes more efficiently. The most prominent approaches on this field are the systematic reduction technique by Peters and Williams, the computational singular perturbation method by Lam, and the ILDM technique introduced by Maas and Pope. For a short review of these methods we refer to [1]. While these works represent already significant improvements in the modeling of combustion processes, according to Polifke et al. [1] they are still of limited applicability for use within large scale, three-dimensional CFD computations due to their numerical complexity as well as their size, resulting in high computational cost.

To describe a combustion process by global kinetics, basically two steps have to be undertaken [2]. First, a set of suitable global reactions has to be found which is expected to be capable of reproducing the detailed mechanism to a high degree. After that, the rate coefficients appearing in these reactions have to be optimized in order to deliver the best possible fit against corresponding detailed data. In recent years the use of simplified global mechanisms in generalized Arrhenius form, optimized by means of genetic algorithms (GAs), was found to be particularly suitable for the task at hand. An extensive review of activities undertaken so far in this area is given in the paper of Elliott et al. [2].

The present paper deals with the optimization of reaction rate coefficients of global 2- and 3-step mechanisms in order to reproduce ignition delay time and temperature profile for self ignition of lean premixed hydrocarbon combustion at high temperatures, as it occurs in many practical applications, e.g. internal combustion engines or gas turbines with reheating stages. On these conditions the governing parameters to describe flame stabilization are no longer the effects of laminar flame speed and diffusion, but the ignition delay time of the fuel-air-mixture, see Brandt et al. [3]. While Westbrook and Dryer [4] derived global 2- and 3-step mechanisms which predict laminar flame speeds (s_L) for premixed and non-premixed combustion at lower temperatures quite well, attempts to predict τ_{ign} at higher ignition temperatures (> 1100 K) with these mechanisms are less promising. The reason for this behavior will be discussed in the next section.

The optimization routine presented here makes use of a so called "nested GA". The advantage of genetic algorithms with respect to traditional gradient based methods is that they are especially adapted for optimization problems with highly complex fitness functions and multiple degrees of freedom, as they are inherent to the optimization problem at hand. On these conditions traditional gradient based algorithms are often difficult to implement and likely to fail.

The paper is organized as follows: First, the specific objectives of the present approach are outlined. Next, some basic equations of reaction kinetics are introduced. After some general aspects of genetic optimization, the structure of the nested GA and its implementation for the current optimization task will be described. Finally, optimization results of 2- and 3-step mechanisms and their applicability on conditions off the design-point will be shown.

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Specific Objectives

According to Polifke et al. [1], reduced 2- or 3-step reaction mechanisms are well suited for use within CFD codes for the computation of turbulent reacting flows. A method was presented which makes use of a GA optimizer to fit reaction rates of a simplified mechanism to data of an underlying detailed mechanism. Species formation rates, temperature profile and laminar flame speeds computed from the optimized reaction rates showed promising results. For more details as well as limitations of this approach the reader is referred to [1] and [2].

For the task at hand, i.e. the prediction of τ_{ign} for combustion at high temperatures, though, the approach used by Polifke et al. [1] is less suitable. Like other methods of the kind, it aims more towards the prediction of laminar flame speeds and species concentration profiles. For an accurate prediction of s_L , the reaction rates of the global mechanism have to be optimized over a wide temperature range (in particular near the adiabatic flame temperature), since they dominate the overall velocity of the combustion process. When applied for the calculation of τ_{ign} , though, the point in time where the reaction begins is of particular importance. This is in turn not dependent on an accurate reproduction of reaction rates over the whole temperature range of the reaction. Therefore, within the current approach we do not try to optimize the Arrhenius rate coefficients in order to reproduce reaction rate expressions, but to fit ignition delay time as well as temperature profile of global mechanisms directly to the corresponding data obtained from a detailed mechanism.

For given operating conditions, i.e. fuel composition, initial temperature, equivalence ratio, pressure, and a given global mechanism, the optimization tool should be able to provide a set of rate coefficients which reproduces τ_{ign} and temperature profile of the detailed mechanism. The GA optimizer used by Polifke et al. [1] was developed further into a nested GA, whose capability of solving highly complex optimization problems should be improved with respect to simpler GAs. In order to provide an efficient optimization tool, the calculations should be easy to perform and computation time should remain within reasonable limits. Finally it has to be found out if the off-design applicability of global mechanisms can be improved.

Governing Rate Expressions

For a mechanism consisting of N species and L elementary reactions, the equations describing the mechanism can be expressed as:

$$\sum_{i=1}^N \nu_{ij}' X_i \leftrightarrow \sum_{i=1}^N \nu_{ij}'' X_i, \quad \text{with } j = 1 \dots L, \quad (1)$$

where ν_{ij}'' are the stoichiometric coefficients for the i th species in the j th reaction on the products' side and ν_{ij}' the corresponding coefficients on the reactants' side.

The chemical symbol of the i th species is denoted by X_i . The net reaction rates r_j for each of the L elementary reaction are:

$$r_j = k_{fj} \prod_{i=1}^N [X_i]^{\nu_{ij}'} - k_{rj} \prod_{i=1}^N [X_i]^{\nu_{ij}''}, \quad (2)$$

where k_{fj} and k_{rj} are the forward and backward Arrhenius-coefficients of the j th reaction:

$$k_j = A_j T^{n_j} \exp\left(\frac{-E_{A_j}}{RT}\right). \quad (3)$$

In eq. (3) A is called pre-exponential factor, n the temperature exponent, and E_A the activation energy of the reaction. The net formation rate $\dot{\omega}_i$ for each species and the molar heat release rate \dot{q} can be expressed as:

$$\dot{\omega}_i = \sum_{j=1}^L \nu_{ij} r_j, \quad \text{with } \nu_{ij} = \nu_{ij}'' - \nu_{ij}', \quad (4)$$

$$\dot{q} = - \sum_{j=1}^L h_j r_j, \quad (5)$$

where h_j denotes the change of enthalpy in the j th reaction when the reactants have completely been transformed into products. It can be obtained by forming the weighted sum over the standard state molar enthalpies H_i of all participating species:

$$h_j = \sum_{i=1}^N \nu_{ij} H_i. \quad (6)$$

While for elementary reactions the species concentration exponents ν_{ij}' and ν_{ij}'' are equal to the stoichiometric coefficients of the participating species, this is in general not the case for global reactions. Replacing the integer concentration exponents of the forward reaction ν_{ij}' with free parameters a_{ij} and inserting eq. (3) in eq. (2), the forward reaction rate of the j th global reaction reads:

$$r_j = A_j T^{n_j} \exp\left(\frac{-E_{A_j}}{RT}\right) \prod_{i=1}^N [X_i]^{a_{ij}}. \quad (7)$$

By inserting eq. (7) in eq. (4) and (5), respectively, the species formation and heat release rates can be calculated. Within the computations only forward reaction rates (see eq. (7)) were used in order to avoid numerical problems such as negative species concentrations and convergence problems of the ODE solver. Consequences arising from this simplification will be discussed in the remainder of the paper.

Self ignition of a homogeneous gas mixture can be modeled using a plug-flow type reactor. To obtain the

time dependent values of species concentration and temperature profile of the reaction, the temporal derivatives of temperature and species mass fraction have to be calculated from the heat release and species formation rates of the mechanism:

$$\frac{dT}{dt} = \dot{q} \frac{1}{c_p \rho}, \quad (8)$$

$$\frac{dY_i}{dt} = \dot{\omega} \frac{M_i}{\rho}, \quad (9)$$

where c_p and ρ denote the specific heat capacity at constant pressure and the density of the mixture, respectively. M_i represents the molar mass of the i th species and Y_i its mass fraction.

Optimization of Rate Coefficients using a Nested Genetic Algorithm

Genetic algorithms (GAs) are optimization algorithms that imitate evolutionary processes as found in nature. It is common practice to use the keywords used in biology to describe the characteristics of GAs. Usually a GA consists of a “population” of “individuals”, who possess genetic properties in the form of “chromosomes”. In a first step the quality of the individuals with respect to the optimization target is rated, which is done by evaluating an object or cost function. In a “selection” step the “fittest” individuals are chosen to become the parents of the next generation. According to Rechenberg [5], a very important characteristic of GAs is their capability of self-adaption, which means that the algorithm controls its own methods according to the requirements of the optimization process. This makes them particularly suitable for optimization problems with highly complex fitness landscapes, where traditional gradient based optimization methods often tend to get stuck on local extrema. Moreover, GAs do not require the knowledge of gradients of the fitness function, which is useful in cases where the computation of gradients is difficult or impossible. For the optimization of reaction rate coefficients, GAs have been successfully employed in a variety of applications so far, see [2].

Polifke et al. [1] used a $(\mu+\lambda)$ -GA developed by Rechenberg [5], where a population of μ parents and λ children evolves through a sequence of generations. While this GA provided promising results for the optimization approach used by Polifke et al. [1], it turned out to be of limited reliability for the task at hand. In some cases the evolution got stuck on local extrema of the fitness surface and did not provide the desired optimum solutions. To overcome this problem, the GA was extended to a so called “nested GA”. While the original GA optimized the individuals of one single population, the nested GA optimizes many populations of individuals. Using the notation introduced by Rechenberg [5], the algorithm may be defined as:

$$\left[\mu' / \mu' + \lambda' (\mu / \mu + \lambda)^\gamma \right]^{\gamma'} - \text{GA}. \quad (10)$$

On onset of optimization, there are μ' “parent populations”, each consisting of μ individuals. In a next step, λ' “child populations” are formed by selecting $\lambda' \cdot \mu$ individuals at random from all μ' populations. After that, all λ' children populations perform γ isolated $(\mu/\mu + \lambda)$ -optimization cycles. The term μ/μ indicates that the chromosomes to form a new child are selected at random from all μ parents of the population. Once all λ' children populations have performed γ isolated optimization cycles, the μ' best populations are selected to become the new parent populations. The whole optimization process is repeated γ' times. For further details on the GA at hand, the interested reader is referred to [5] and [6]. A benefit of the nested GA is its ability to explore different regions of the fitness landscape by different populations who evolve independently. This is especially useful when highly complex fitness functions with numerous local extrema are investigated. Where a GA consisting of a single population might get stuck on a local optimum, the nested GA offers the possibility to compare optimization results from different populations and therefore is able to “concentrate” on regions of interest. Thus, the convergence radius of the GA is no more predefined by the initial parameters of one single population.

When applying the GA described above to the current optimization task, the strategy can be outlined as follows: In order to derive rate coefficients for a global mechanism, first a set of detailed data, which models the combustion process in the desired operating point, has to be provided. To compute reference data for τ_{ign} and temperature profiles, the SENKIN computer program by Lutz et al. [7] was used, which is part of the CHEMKIN package [8]. It calculates the time dependent reaction progress for combustion of a homogenous gas mixture in a closed system. The underlying detailed kinetics model for methane combustion was the GRI-Mech 3.0 mechanism [9] with 325 elementary reactions and 52 species. For a given set of initial conditions, i.e. initial temperature T_0 , constant pressure p and equivalence ratio ϕ of the mixture, the temperature and species concentration profiles are computed for a reactor runtime divided in N_t representative time steps ($k = 1 \dots N_t$). Then the GA is employed to optimize the reaction rate coefficients A_j , n_j , E_{A_j} and a_{ij} , ($i = 1 \dots N$, $j = 1 \dots L$) of the global mechanism in order to reproduce τ_{ign} as well as the temperature profile of the detailed mechanism.

Since there are two optimization targets, τ_{ign} and temperature profile, an appropriate definition of the cost function, which should be able to take into account both values equally, is crucial. The following equation shows the function used to calculate the overall fitness f of a parameter set:

$$f = \left\langle w_T \left| \ln \left(\frac{T_{k,\text{det}}}{T_{k,\text{opt}}} \right) \right| + w_{\tau_{\text{ign}}} \left| \ln \left(\frac{\tau_{\text{ign},k,\text{det}}}{\tau_{\text{ign},k,\text{opt}}} \right) \right| \right\rangle. \quad (11)$$

The first term represents the logarithmic deviation of the detailed mechanism's reaction temperature at the k th time step with respect to the temperature of the global reaction at this point. The second term represents the logarithmic deviation of τ_{ign} at the k th time step in the same manner. Ignition delay time is defined as the point in time when the temperature of the reaction reaches 50% of its overall rise. Absolute values of the logarithmic terms are used in order to obtain positive fitness values only. By weighting factors w_T and $w_{\tau_{\text{ign}}}$ the impact of the logarithmic expressions on the fitness can be balanced. For the computations presented here both weighting factors were set to unity. Averaging $\langle \dots \rangle$ the deviations over all N_t time steps provides the overall fitness of the parameter set. Note that the logarithmic terms are zero in case of a perfect match between detailed and global values of τ_{ign} and temperature profile. In order to reach an optimum solution, the cost function has to be minimized. Polifke et al. [1] used a fitness function similar to the one shown above. Their function basically averaged the logarithmic deviation between the global and detailed reaction rates over a given temperature range. It has to be mentioned that the present software is not only able to use temperature profile in conjunction with ignition delay time as optimization targets, but any species concentration profile can be used instead of temperature. This possibility to perform so called "multi-objective" optimization is another advantage of GAs over other optimization methods. Results obtained from different combinations of optimization targets are beyond the scope of the present work, though.

In order to use τ_{ign} and the temperature profile (or any species concentration profile) as optimization targets directly, the governing equations eq. (3) to (9) have to be computed within each call to the cost function. Since, especially with nested GAs, the number of cost function computations can be very high (depending strongly on the number of populations, individuals per population, overall repetition of the optimization strategy etc.), a powerful and fast ODE solver was required to perform this task. The C-language program CVODE by Cohen and Hindmarsh [10] was found to be suited for this purpose. To achieve a further reduction of computation time, a data reduction technique was implemented which reduces the overall number of data points (i.e. the number of time steps evaluated by SENKIN and CVODE computations) to a number of representative time steps N_t . It also permits to adjust the density of reference data points along the optimization target's gradient. If one is interested in an accurate reproduction of the temperature profile in the surroundings of the point of ignition, for example, the density of reference data points may be increased in regions with high temperature gradients. Areas with lower temperature gradients, e.g. on onset of

the reaction, obtain less reference data points and thus have less impact on cost calculation.

Regarding computational cost, it has to be admitted that the optimization tool, especially due to the complexity of the nested GA, which by its nature requires a higher number of calls to the fitness function than a simple GA, involves higher computational effort than simpler optimization strategies. Moreover, the computation of the cost function is by itself an elaborate task due to the stiff differential equation computations. All results shown in this paper were obtained using the following values to operate the GA: $\mu' = 5$, $\lambda' = 10$, $\gamma' = 3$, $\mu = 12$, $\lambda = 30$, $\gamma = 10$. With 9000 evaluations of the cost function the overall computation time on a 1.8 GHz machine was about 15 minutes for a 2-step mechanism, which is still in acceptable limits.

Results and Discussion

Computations were conducted for various global 2- and 3-step mechanisms. Table 1 contains the reaction rate coefficients of the global mechanisms discussed in this section. The 2-step mechanism for methane combustion described here uses CO as an intermediate and can be written as:

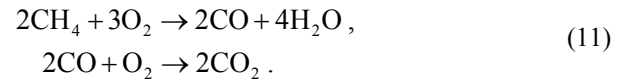


Fig. 1 shows the temperature and species profiles for the given 2-step mechanism at a pressure of 16.7 bar. The elevated pressure was chosen since the operating conditions in the second combustion chamber of a gas turbine with reheating stage were to be modeled. Regarding the point of ignition time, it can be seen that both the detailed and the global mechanism are in good agreement.

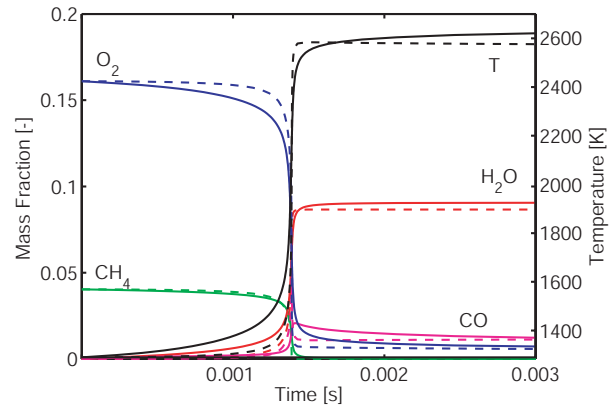
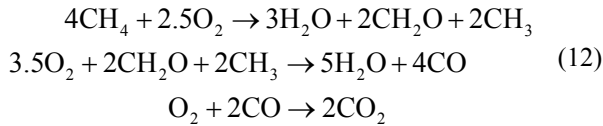


Fig. 1: Temperature and species profiles of detailed (---) and global (—) 2-step mechanism against reaction time. Initial conditions: $p = 16.7$ bar, $T_0 = 1290$ K, $\phi = 1$. Reaction rates taken from mechanism 2step_4.

For species and temperature profiles the fits are satisfactory, yet some deviations can be observed. The global mechanism's temperature profile begins to rise shortly after onset of the reaction. At the same time, oxygen and methane concentrations begin to decrease

below the corresponding detailed values. In the same manner water is formed right after the beginning of the reaction. Obviously, the global mechanism is not fully capable of reproducing the temperature and species profiles of the detailed mechanism, where constant temperature and species concentration on onset of the reaction are maintained over a longer period of time. The effect of immediate heat release and reactant species consumption could be observed for all global mechanisms, both 2-step and 3-step, which were optimized so far. At lower pressures, the deviation from the detailed mechanism's behavior was even more pronounced (not shown). Towards the end of the reaction one can see that the end temperature of the global mechanism is higher than the reduced mechanism's equilibrium temperature. This arises from the fact that only forward rates (see eq. (7)) are used to calculate the reaction progress. Neglecting backward reactions, a chemical equilibrium state can not be reached, and the amount of heat which is normally consumed by dissociation processes in a detailed mechanism results in a higher end temperature for the global mechanism. In the same manner the species concentration of H_2O at the end of the reaction is overpredicted by the global mechanism. From another 2-step mechanism using CH_2O and CH_3 as intermediates (not shown), similar results were obtained.

For optimization of 3-step mechanisms the following reaction scheme, using CH_2O , CH_3 and CO as intermediates, will be discussed:



Optimization results (not shown) using this mechanism at elevated pressure delivered equally good results for the prediction of τ_{ign} as shown in Fig. 1. The problem of immediate heat release right from the beginning of the reaction was more pronounced, though. To remedy this problem it was tried to inhibit the start of the global mechanism's first reaction by the use of so called promoted species. This is done by choosing an

intermediate species of the first reaction and adding it to the initial fuel mixture in a very low concentration (approx. 10^{-9}). The forward rate of the reaction is then calculated by including the promoted species' concentration and concentration exponent in eq. (7):

$$r_j = A_j T^{n_j} \exp\left(\frac{-E_{A_j}}{RT}\right) \left(\prod_{i=1}^N [X_i]^{a_{ij}}\right) [X_{j,prom}]^{a_{j,prom}}, \quad (13)$$

where $X_{j,prom}$ and $a_{j,prom}$ are the promoted species' concentration and concentration exponent, respectively. Since the initial concentration of the species is very low, also reaction rates can be kept down.

Fig. 2 shows species and temperature profiles for a parameter set optimized at atmospheric pressure where CH_3 is used as promoted species to inhibit the onset of the first reaction.

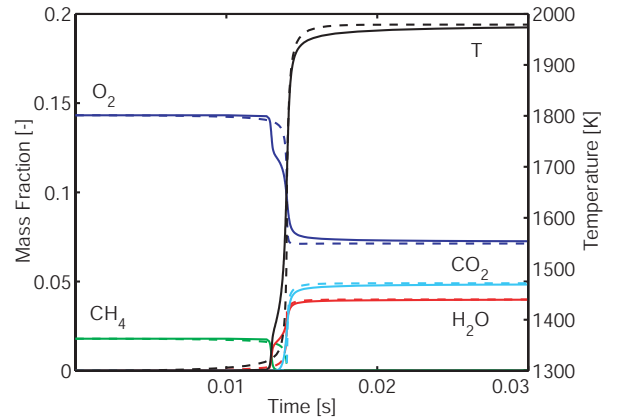


Fig. 2: Temperature and species profiles of detailed (- -) and reduced (-) 3-step mechanism against reaction time. Initial conditions: $p = 1$ bar, $T_0 = 1300$ K, $\phi = 0.5$. Reaction rate coefficients from 3stepF_3, CH_3 is used as promoted species to control the rate of the first reaction.

It can be seen that the initial temperature rise as well as the consumption of reactant species can be effectively kept down at the beginning of the reaction. Shortly before ignition of the detailed mechanism, though, the global temperature profile shows a sharp bend and a significant amount of heat is released in a short period of time. From the CH_4 and O_2 profiles one can see that

Name	T_0 [K]	p [bar]	ϕ	Species concentration exponents					$\log_{10}(A)$	n	E_A/R
				CH_4	O_2	CO	CH_2O	CH_3			
2step_4	1290	16.7	1	0.8603	2.9483	0	0	0	15.913	0.7218	36084
				0	2.6911	2.2800	0	0	15.893	0.7254	22521
2step_3	1290	1	0.66	1.0430	0.4611	1.7318	0	0	15.579	0.8449	15279
				0	1.1479	1.6858	0	0	15.590	0.5751	30826
3stepF_4	1290	16.7	0.5	1.8838	0.0162	0	0	1.3145	15.618	0.9602	26150
				0	2.8279	0	1.6410	1.2582	15.562	0.9604	9089
				0	2.9596	1.4645	0	0	15.487	1.2357	30514
3stepF_3	1300	1	0.5	1.6189	1.9197	0	0	1.4843	15.050	1.8006	12087
				0	0.7481	0	1.8723	1.3019	15.607	2.5245	34149
				0	0.8798	1.5511	0	0	15.715	0.9887	35042

Table 1: Reaction Rate Coefficients for Optimized 2- and 3-step mechanisms at different design-points

the first reaction of eq. (12) occurs too early with respect to the detailed mechanism. The second and third reaction of the mechanism progress more smoothly and show satisfying agreement with the detailed data. Further optimization runs, using promoted species for 2-step and 3-step mechanisms, delivered similar results (not shown). While the use of promoted species seems to be well adapted to inhibit reaction rates over a certain period of time, it turned out to be difficult to match the detailed mechanism's temperature and species profiles completely.

The quality of a global mechanism is not only determined by its capability of reproducing the underlying detailed mechanism at the design point, but also by its ability to deliver satisfying results when used on off-design conditions. In order to validate the global mechanisms' quality in this context, 2- and 3-step mechanisms were tested for varying values of initial temperature and equivalence ratio. In Fig. 3 results are shown for two 2-step mechanisms and two 3-step mechanism optimized at atmospheric and elevated pressure.

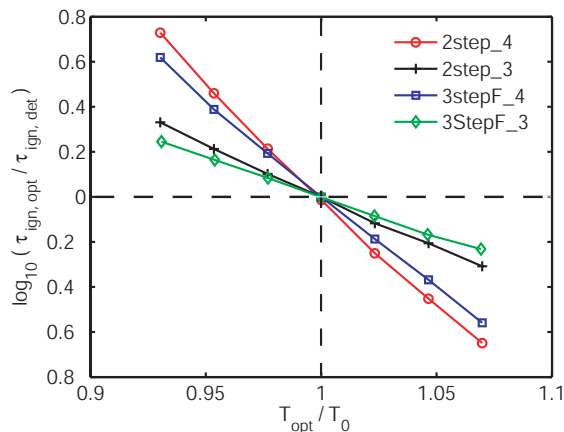


Fig. 3: Deviation of ignition delay time predicted by reduced mechanisms from τ_{ign} of detailed mechanism for varying values of T_0 .

From the logarithmic representation one can see the behavior of global mechanisms in off-design operation points. For initial temperatures below the design point, τ_{ign} predicted by the global mechanism is higher than predicted by the detailed mechanism. For initial temperatures higher than the design point, the contrary behavior is observed. For a perfect match between detailed and reduced ignition delay times over the whole temperature range, the logarithmic expression on the ordinate is zero, resulting in a horizontal line. If the deviation reaches unity, τ_{ign} is over- or underpredicted by one order of magnitude. Mechanisms 2step_4 and 3stepF_4 were both optimized at elevated pressure and show the strongest deviation at varying initial temperatures. Note that mechanism 3stepF_4 was optimized using CH_3 as promoted species to control the reaction rate of the first reaction. Compared to other optimization results (not shown), it was seen that the use of promoted species could improve the fit of a mechanism's species and temperature profiles at the

design point, while this benefit was not observed for the prediction of τ_{ign} at off-design operating points. Mechanisms 3stepF_3 and 2stepF_3, both using promoted species, were optimized at atmospheric pressure and show better results for varying initial temperatures. At lower pressures the use of promoted species did improve the deviation of τ_{ign} at off-design operating points. For varying values of ϕ around the design point (not shown) similar results were obtained.

Conclusions

Scope of the present work was the development of a computational tool to derive reaction rate coefficients of global 2-step and 3-step mechanisms for self ignition of lean premixed methane-air mixtures at high temperatures in order to predict ignition delay times. A nested genetic algorithm was developed and could be successfully employed to carry out the optimization task at hand. It could be shown that global 2- and 3- step mechanisms are able to reproduce τ_{ign} , temperature and species profiles at the design point well. The use of promoted species to improve this agreement was demonstrated. When applied for the prediction of ignition delay times at off-design operating points, all global mechanisms showed notable deviations. Compared to results obtained from global mechanisms of other origin [4] [1], though, an improved behavior for the prediction of ignition delay time could be observed.

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