

Reduction of a Detailed Kinetic Model for the Ignition of Natural Gas Mixtures at Gas Turbine Conditions

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Abstract

Natural gas is the primary fuel for industrial gas turbines. Although natural gas is mostly methane, its composition varies. Detailed reaction mechanisms were developed to describe the ignition delays for mixtures with higher hydrocarbon content. The size of this detailed chemical kinetic model is too large to be used in CFD calculations. The aim of this study was to reduce the number of species and reactions to get a mechanism small enough to use in CFD calculations. A 39-species reduced mechanism was obtained which provides 3.9% average deviation in the ignition delay times for lean and stoichiometric mixtures containing 10% propane / 90% methane as fuel, in the pressure interval 10–40 atm and temperature range 876–1465 K.

Introduction

Natural gas is the primary fuel for industrial gas turbines [1], which currently provides about one quarter of the world's primary energy supply, and is expected to remain a significant source of energy until 2030. Natural gas has a low greenhouse gas signature, is energy efficient and is easy to use in that the infrastructure needed is already built. Although natural gas is mostly methane (CH₄) its composition varies depending on its origin, extraction, and transport processes [2]. The variation in fuel composition is expected to increase due to the growing usage of non-traditional gas sources. Consequently, fuel-flexible gas turbines are of interest to the power generation and combustion research communities. This variation can impact the performance of dry, low-emission industrial gas turbine engines through variation in the autoignition delay time, flame dynamics, and flame speed [3-5]. Ignition delay time is a fundamental parameter, because the residence times in the premixed section of the combustor for the premixed fuel-air compositions need to be below the mixture's autoignition time at a given temperature and pressure [6]. The higher-order hydrocarbon (for example ethane (C₂H₆), propane (C₃H₈), butane (C₄H₁₀), etc.) content of the natural gas requires the application of detailed chemical kinetic models describing the oxidation of not only methane, but also the high hydrocarbons. Curran and co-workers recently developed a detailed reaction mechanism for the description of the oxidation of such mixtures [7-9]. This mechanism reproduces the ignition delays for different mixtures at a wide range pressure intervals (1–50 atm) over the temperature range 740–1550 K quite well. However, the size of this detailed chemical kinetic model is far larger (above 200 species) than it can be used directly in Computational Fluid Dynamics (CFD) calculations.

The simulation speed can be increased using reduced mechanisms. Almost all published detailed reaction mechanisms contains redundant species and reactions [10]. There are several methods for mechanism reduction [10-32]. One type eliminates the redundant species and reactions, but maintains the level of elementary reactions. This type of mechanism re-

duction has several benefits, e.g. the simulation time may decrease significantly, the reduced mechanism remains a subset of the original full mechanism, and hence it is easier to understand the chemical processes that take place.

Our aim was to reduce the number of species and reactions to get a reduced mechanism small enough to be used directly in CFD calculations and to provide a small but still accurate input mechanism for other reduction methods that can accelerate the simulations further.

Specific Objectives

In reacting flow simulations the differential equations coming from both the fluid dynamics and chemistry are solved, which makes them computationally very expensive. There are several different CFD codes [33], but most of them can only handle the chemistry in a very simplified way. They use only one global reaction or a set of severely condensed reaction steps. For several applications this simplification is acceptable, but gas turbine combustor designers have found that they cannot sacrifice chemical accuracy for resolution in geometry and flow when they simulate ignition delay times or the formation of pollutants. For such calculations researchers use special CFD software which permits the use of a detailed chemical kinetic mechanism (for example Fluent [34] or CHEMKIN-CFD [35] coupled with a CFD software). There is no theoretical limitation of the number of species utilized in the detailed mechanism calculations; however the simulation time becomes unacceptably long. This is why the practical 50 species limit was introduced in the code of Fluent. There is no species limit in CHEMKIN-CFD, but it is not practical to include reaction mechanisms that contain more than 50 species.

The recently developed detailed reaction mechanisms for the description of the oxidation of methane/higher hydrocarbon mixtures contain more than two hundred species and more than a thousand reactions [7-9]. Thus, these mechanisms cannot be used directly in CFD calculations. Application of mechanism reduction techniques on these mechanisms may

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lead to applicable size, but still accurate mechanisms. There are several methods in the literature for mechanism reduction (see e.g. [10-32]). Some produce subsets of the original mechanism, while others substitute a part of the original mechanism by lumping species/reactions and others use time-scale analysis to remove fast time-scales to accelerate the simulations. Our aim was the diminution of the number of species and reactions to get a reduced mechanism which is small enough to include directly into CFD calculations for each regime and provide mechanisms applicable for conditions covering more than one regime.

In this work we focused on the ignition delay calculations. The ignition delay times can vary by several magnitudes from a few μs to a couple hundred ms when the circumstances change. The ignition delay time was the final target in the mechanism reduction. Practically, the prediction of the ignition delay time within 10% relative error can be considered to be very accurate. Therefore, a 10% relative error in the ignition delay time was chosen as threshold for the acceptance of a reduced mechanism. We wanted to keep the original species and elementary reactions in the reduced mechanisms, so species elimination methods were applied. The analysis was carried out in three stages. At the first, reduced mechanisms were created for one or a few selected representative cases (scenarios) of each regime. At the second stage, reduced mechanisms were developed valid for each regime based on the results of the first stage. At the third, the aim was to find reduced mechanisms valid for groups of regimes and even for all cases included in the analysis.

Simulations

The calculations in this study are based on the

regime	p/atm	CH ₄ /C ₃ H ₈	ϕ	T / K	RCM	ST
1	10	90/10	0.5	1025-1099	Yes	No
2	20	90/10	0.5	903-1037	Yes	No
3	30	90/10	0.5	1252-1369	No	Yes
4	40	90/10	0.5	876-909	Yes	No
5	10	90/10	1.0	1281-1465	No	Yes
6	20	90/10	1.0	1117-1271	No	Yes
7	10	70/30	1.0	917-1375	Yes	Yes
8	30	70/30	1.0	751-1503	Yes	Yes
9	7	70/30	3.0	1167-1425	No	Yes
10	20	70/30	3.0	740-830	Yes	No
11	30	70/30	3.0	734-1352	Yes	Yes

Table 1 Regimes used for the mechanism reduction

experimental results published in the paper of Healy et al. [2]. This paper contains ignition delay time data for methane/propane mixtures at several different pressures, methane/propane ratios and equivalence ratios relevant to gas turbine conditions. Ignition delay times were measured using rapid compression machine at lower temperatures and using shock tube at higher temperatures. These experiments covered temperature interval 713–1465 K, pressure interval of 7–40 atm, methane/propane ratios 70/30 and 90/10 and equivalence ratios 0.5, 1.0, 2.0 or 3.0 giving 11 different regimes, see Table 1. The overall number of cases used for the mechanism reduction was 174 and 19 representative cases (scenarios) were selected from them for mechanism reduction. Details of the scenarios can be found in Table 2. The system can be approximated as being adiabatic and of constant volume. Simulation were carried out with code tibox, (part of the program package used for the mechanism reduction), which

regime	scenario	pressure / atm	temperature / K	Initial composition in mole fractions				
				CH ₄	C ₃ H ₈	O ₂	Ar	N ₂
1	1	9.79	1032.6	0.0393	0.0044	0.2008	0.7555	0.0000
	2	10.37	1096.2	0.0393	0.0044	0.2008	0.7555	0.0000
2	3	21.86	915.5	0.0393	0.0044	0.2008	0.7555	0.0000
	4	19.63	952.9	0.0393	0.0044	0.2008	0.7555	0.0000
	5	19.97	1034.4	0.0393	0.0044	0.2008	0.7555	0.0000
3	6	30.90	1294	0.0393	0.0044	0.2008	0.7555	0.0000
4	7	39.44	876.5	0.0393	0.0044	0.2008	0.3778	0.3778
	8	38.90	907.4	0.0393	0.0044	0.2008	0.3778	0.3778
5	9	6.84	1318	0.0753	0.0084	0.1924	0.0000	0.7239
6	10	24.32	1117	0.0753	0.0084	0.1924	0.0000	0.7239
7	11	9.60	918.8	0.0473	0.0203	0.1958	0.4420	0.2947
	12	9.67	959.7	0.0473	0.0203	0.1958	0.4420	0.2947
	13	7.89	1244	0.0473	0.0203	0.1958	0.0000	0.7367
8	14	30.26	845	0.0473	0.0203	0.1958	0.36835	0.36835
	15	29.10	1280	0.0473	0.0203	0.1958	0.0000	0.7367
9	16	7.56	1291	0.1249	0.0535	0.1725	0.0000	0.6490
10	17	19.66	779	0.1249	0.0535	0.1725	0.0000	0.6490
11	18	29.86	787.1	0.1249	0.0535	0.1725	0.5192	0.1298
	19	27.10	1144	0.1249	0.0535	0.1725	0.0000	0.6490

Table 2 Selected scenarios for the mechanism reduction

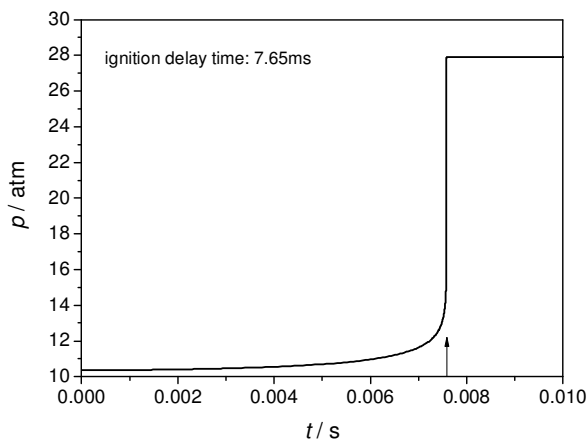


Fig. 1. Definition of the ignition delay time. Pressure profile in scenario 2.

predicts same ignition delay times as CHEMKIN-PRO [36].

We defined the ignition time as the point at which the time derivative of the pressure is at a maximum, see Fig. 1.

Curran and co-workers recently developed a detailed reaction mechanism for the description of the oxidation of such mixtures [7-9]. The latest version of the C4 mechanism [37] (it contains 230 species up to 4 carbon atoms and 1327 reversible reactions) was used as input of the mechanism reduction.

Methods

Reducing the full mechanism using species elimination methods allows us to keep the original species and elementary reactions in the reduced mechanisms. This means that the reduced mechanisms are subsets of the original mechanism, and no new species and reactions are allowed. In this paper we applied recently developed methods for the mechanism reduction.

A new method, the Simulation Error Minimization Connectivity Method (SEM-CM) [38] was published recently which provides a massive decrease in the number of species and reactions, but keeps the reduced mechanisms within the prescribed accuracy. The SEM-CM method is based on the analysis of the Jacobian. The error in concentration profiles of the important species during the reduction process are minimized directly. Several reduced mechanisms are built from starting sets of the important species by adding small sets of species. Set addition is controlled by the depth level of the analysis. The important species set was determined as the major species during the simulations and the concentrations of these species were used in the error functions. For the analysis and error calculations 40 points (in scenarios 17 and 18 60 points) were taken in uniform distribution in a time interval including the ignition delay time. The starting time point was placed at time when the major mole fractions start to change significantly (beside this 0s was included in all cases).

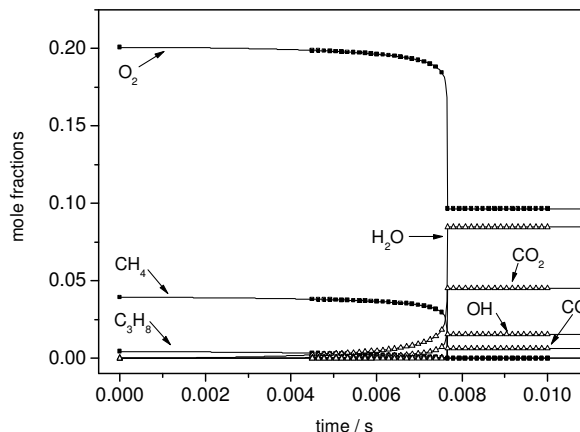


Fig. 2. Points for the analysis and the error calculations in scenario 2.

The last point was placed after the ignition time to get significant change in the error function when the ignition becomes slower. The placement of the points varied from scenario to scenario. Fig. 2 shows how the points were placed in scenario 2.

In this work a combination of two directed relation graph methods (the “DRG with Error Propagation” method (DRGEP) [30] and the “DRG-aided sensitivity analysis” method (DRGASA) [27]) were also combined to identify the unnecessary species.

The DRG methods investigate the reaction graph (principally the system of kinetic differential equations). The DRGASA may significantly improve the results of the DRG method by the removal of those species whose omission causes only minor increase in the simulation error of the important species. The DRGEP method is based on the DRG method, but measures the interaction of species in a more effective way. It is also possible to define DRGEPASA method (analogously to DRGASA) based on the results and the interaction coefficients of the DRGEP. The DRGEP + DRGEPASA method provides better results than DRG + DRGASA and DRGEP methods.

These methods were implemented in a FORTRAN package developed by Nagy [39]. A FORTRAN package containing the SEM-CM method is freely available from the internet [39]. This package does not allow the direct use of the ignition delay time as a target. However, the ignition delay time is related to the calculated pressure–time profile, and the pressure is determined by the concentration of the major species. Consequently, the initial important species set was selected as the set of target species.

The SEM-CM mechanism reduction method was applied for 19 cases which covers all regimes. The process was repeated for all cases with depth levels 1, 4, 16, 256, 1024 (and all, if it was needed). Calculations at higher depth level utilized the results of all previous levels. This can be summarized in notations: 1, ...+4, ...+16, ...+256, ...+1024. For a few cases this analysis provided quite large reduced mechanisms (see the next section). In these cases, SEM-CM and DRGEPASA methods were applied one after the other till results cannot be improved further. The ignition delay times were calculated with the original mecha-

nism and the reduced mechanisms and the differences were determined automatically. A reduced mechanism was accepted as being accurate enough when the calculated ignition delay deviated by less than 10% compared to the baseline, detailed mechanism calculation. Reduced mechanisms developed for one scenario were tested for others in terms of ignition delay time. Beside, SEM-CM analyses were done for regimes, including two or three scenarios simultaneously. This should lead to accurate ignition delay times for multiple cases, but when more scenarios are considered it is much more difficult to obtain a small reduced mechanism. Using these techniques common reduced mechanisms were determined which provided the required accuracy for multiple cases.

Results and Discussion

For the mechanism reduction, selection of important species to be included into the error function was required. The coincidence of the rapid pressure increase (ignition) with the dramatic change in concentration profiles of major species enabled us to use the concentrations of these species in the error functions. The accuracy of a reduced mechanism in reproducing ignition times is only indirectly related to the accuracy of its concentration profiles. The program package calculates two error measures from the concentration profiles of the important species, (i) the overall maximum relative error (δ_{MAX} , refers to the maximum relative deviation) and (ii) the root mean square relative errors of important species (δ_{RMS} , refers to the average relative deviation). In order to decide which error measure correlates the most/best with the error of the ignition delay time, the profiles of a major species were plotted versus time for reduced mechanisms with different δ_{MAX} and δ_{RMS} errors, Fig. 3.

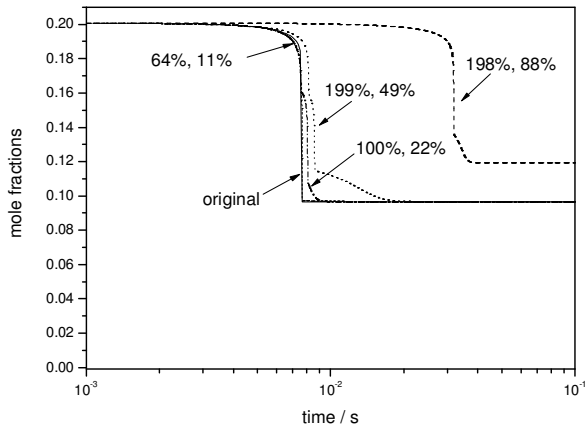


Fig. 3. Change of oxygen concentration in time while the δ_{MAX} and δ_{RMS} errors changes in scenario 2.

It can be seen that the δ_{MAX} cannot be used for the prediction of accurate ignition delay times because this measure can remain the same while the ignition delay time changes significantly.

Applying SEM-CM method several reduced mechanisms were created and tested at a given species number. At each number of species, the reduced mechanism having the smallest δ_{RMS} error was selected. These mechanisms are the most accurate recommenda-

tions of the SEM-CM method at each species number. The δ_{RMS} error of these mechanisms decreased mostly monotonically versus the number of species but in an unsteady way, Fig. 4 for the results obtained in scenario 8.

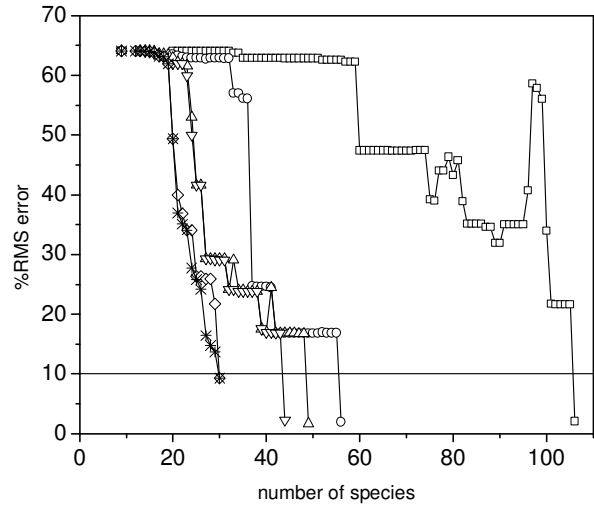


Fig. 4. Species number of the reduced mechanisms at different depth level in the SEM-CM analysis in scenario 8. Depth level 1: \square , ...+4: \circ , ...+16: \triangle , ...+64: ∇ , ...+256: \diamond , ...+1024: $*$.

Increasing the depth level of the analysis the aimed 10% root mean square relative errors of important species can be obtained by less and less species, see the results for all scenarios in Table 3.

It was found that each accepted mechanism also reproduced the ignition delay time within 10% of error in the scenario it was developed for. Smaller mechanisms with higher δ_{RMS} error were also tested with respect to the ignition delays and the smallest one that still reproduces ignition delay times well enough were selected. The numbers of species of the accepted mechanisms for each scenario are shown in Table 3. Each of them provided accurate ignition delay time at their corresponding scenario, but sometimes failed in others. To test it the scenario level accepted mechanisms and others with a lower δ_{RMS} error were tested in all cases. It might seem reasonable to derive a regime level reduced mechanism by taking the union of all of the scenario level reduced mechanisms. However, these very small reduced mechanisms predict accurate ignition delay times for only the corresponding scenario utilizing compensations. Compensation means that the effects of the elimination of more species cancel each other out. Adding more species to this balanced system may lead to significant change in the ignition time. Due to this reason this strategy can not be used to develop regime level accepted mechanisms. To solve this problem mechanism reduction was done including two or three scenarios into the targets in the SEM-CM reduction process. Using these techniques regime level reduced mechanisms were created, see the regime column in Table 3.

For regimes 10 and 11 the reduction failed using both the SEM-CM method alone and using the

		Number of species in the smallest mechanism having less than 10% δ_{RMS} error at a given depth level in the SEM-CM method						Smallest accepted mechanism in the	
		1	...+4	...+16	...+64	...+256	...+1024	scenario	regime
1	1	53	49	23	23	23	23	17	34
	2	57	57	57	27	27	27	19	
2	3	199	48	29	29	29	29	21	21
	4	54	33	29	24	24	24	21	
	5	44	41	22	22	22	22	22	
3	6	76	42	42	42	20	20	17	17
4	7	111	92	28	28	28	28	23	23
	8	107	57	50	45	31	31	23	
5	9	62	27	23	23	21	21	16	19
6	10	204	67	62	33	21	21	17	39
7	11	156	82	28	28	28	28	18	39
	12	123	73	35	31	28	28	20	
	13	138	134	39	39	39	39	19	
8	14	215	164	164	39	39	39	24	
	15	132	77	77	61	61	61	18	
9	16	111	31	29	25	25	25	20	
10	17	213	161	82	34	28	28	24	
11	18	208	208	148	148	>130		34	
	19	98	92	43	28	28	28	20	

Table 3 Change of the species number of the smallest reduced mechanisms having less than 10% δ_{RMS} error in the selected scenarios and the size of the accepted mechanism

DRGEPASA method, too. The mixture in scenario 18 contains 30% propane / 70% methane and shows negative temperature coefficient (NTC) behaviour [40]. It is well known that the chemistry in the NTC region is very complex. This feature was reflected in the difficulty in producing small reduced mechanism under these conditions. Therefore, for scenario 18 DRGEPASA and SEM-CM methods were applied one after the other to get reasonable sized reduced mechanism.

The most widely applicable reduced mechanism contains 39 species valid for all cases in regimes 1, 2, 3, 5, 6, 7 and for two cases in regime 4. For the 2 remaining cases in regime 4 it predicted the ignition delay times within 22% error. This mechanism was able to predict the ignition delay times within 10% error compared to the full mechanism for lean and stoichiometric mixtures containing 10% propane / 90% methane as fuel, in pressure and temperature intervals 10–30 atm and 876–1465 K, respectively. The average error in the ignition delay times using this 39-species reduced mechanism was only 2.5% for these cases. Including regime 4 (40 atm cases) the deviation for all cases with 10% propane / 90% methane mixtures was 3.9% on average. The average calculation speed increased by a factor of 30 considering these cases.

A 39-species reduced mechanism was obtained which provides 3.9% average deviation in the ignition delay times for lean and stoichiometric mixtures containing 10% propane/90% methane as fuel, in pressure interval 10–40 atm and for temperatures 876–1465K. This mechanism contains the following species (and their reactions): H, H₂, O, O₂, OH, H₂O, HO₂, H₂O₂, CO, CO₂, CH₂O, HCO, CH₃O,

CH₃O₂H, CH₃O₂, CH₄, CH₃, C₂H₆, C₂H₅, C₂H₄, C₂H₃, C₂H₂, CH₂CHO, CH₂CO, CH₃COCH₃, CH₃COCH₂, C₃H₈, iC₃H₇, nC₃H₇, C₃H₆, C₃H₅-a, C₃H₅O, IC₃H₇O₂, iC₃H₇O, CH₃CHCO, C₄H₈-1, iC₄H₈, N₂, Ar.

Conclusions

A series of reduced mechanisms have been produced for the accurate description of ignition delay times for methane / propane mixtures under conditions relevant to gas turbines. 19 scenarios in 11 regimes were investigated in the reduction analysis, but the reduced mechanisms were tested in all 174 cases. Scenario and regime level reduced mechanisms were generated which predicted ignition delay times within 10% of those calculated using the full C4 mechanism for each scenario and regime, respectively. A 39-species reduced mechanism was obtained giving accurate ignition delay times for regimes 1–8, which covers all cases containing 10% propane / 90% methane mixtures. The average deviation of the ignition delay times was 3.9%. The calculations were 30 times faster using this mechanism compared to the full C4 mechanism.

More practically, reduced mechanisms for a wider range of temperature, pressure, equivalence ratio and fuel composition would be useful. To produce such, more general reduced mechanism multiple cases have to be included in the mechanism reduction process. In this way the reduced mechanisms will provide accurate ignition delay times for all conditions, but it will also have a significantly larger size. More work is needed in this direction.

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