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Global sensitivity analysis of detailed chemical kinetic schemes for DME oxidation in premixed flames

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Abstract

Detailed chemical kinetic investigations on dimethylether oxidation in one-dimensional premixed flat flames were performed. Local and global sensitivities of the reaction rate constants within selected chemical kinetic schemes were studied using maximum flame temperature, and peak methane and formaldehyde concentrations as predictive target quantities. The global sensitivity analysis was based on the application of high dimensional model representations using quasi-random sampling. First- and second-order sensitivity indices of important reaction steps were determined for fuel rich ($\Phi = 1.49$) and fuel lean ($\Phi = 0.67$) conditions. Differences in the importance ranking for key reactions were found to exist between the selected schemes, highlighting the influence of differences in the key rate constants. Whilst the peak flame temperature was predicted with fairly low uncertainty by both schemes, significant uncertainties were identified in the prediction of the target minor species. Key reaction rates requiring better quantification in order to improve the prediction of methane and formaldehyde concentrations are identified.

Introduction

Cleaner combustion devices based on the utilization of oxygenated fuels provide promising options for the development of lower carbon strategies in the transportation and energy sectors in the near future. Nevertheless, reducing uncertainties in predicted concentrations of minor products from the combustion of ethers or furans still remains a challenging task for combustion modelers and experimentalists. Dimethylether (DME), being a simple candidate for an oxygenated fuel, can serve as a reference case in this context [1].

The availability of accurate and reliable detailed chemical kinetic models of DME oxidation is of key importance for the further development of simplified schemes that could be used for simulating practical combustion devices. The sensitivity of selected predictive targets (e.g. flame temperature, species concentrations, ignition delays) to potential uncertainties within the input data to such schemes can be explored using a range of sensitivity techniques. This helps to identify the most important parameters which determine the accuracy to which key combustion properties can be predicted. These parameters (e.g. rate constants) can then be the subject of more detailed experimental and theoretical studies in order to provide their improved quantification, thus helping to improve the predictive accuracy and robustness of the schemes.

The quasi-random sampling high dimensional model representation (QRS-HDMR) method [2] has proved to be an efficient tool for mapping the relationships between the inputs and outputs of models and therefore can be used to perform global sensitivity analysis of detailed chemical kinetic models. Global sensitivity analysis enables the study of the impact of reaction rates

over their whole range of uncertainty and allows couplings between parameters to be explored. Such information is crucial in order to identify the most important parameters influencing the prediction of the chosen target quantities and provide deeper insight into the complex chemistry involved in DME flames.

Suitable data for chemical kinetic studies of DME oxidation are mostly provided for homogenous systems (e.g. jet-stirred [3] and flow [4,5] reactors). Only a limited number of relevant experimental and modeling studies have been performed for inhomogeneous combustion systems. Laminar flame speed data [6-8], extinction strain rates [8] or ignition temperatures [9] were previously used for model validation and refinement of available chemical kinetic mechanisms for DME oxidation. However, a comprehensive global uncertainty/sensitivity analysis has not yet been performed for such conditions. In order to achieve this goal, simulations of temperature and species concentration profiles were performed for previously experimentally studied atmospheric pressure premixed flat flames of fuel rich ($\Phi = 1.49$) and fuel lean ($\Phi = 0.67$) DME/air mixtures [10].

Specific objectives

In the current work we aim to carry out local and global sensitivity analysis of chemical kinetic schemes for DME oxidation using the experimental setup described by Kaiser et al. [10] as the initial and boundary conditions for the modeling study. Detailed chemical kinetic mechanisms published by Zhao et al. [11] (herein called the “Princeton” scheme) and the skeletal scheme prepared from modifications of [4] (herein called the “LLNL” scheme) were adopted for this purpose. One aim is to establish whether differences

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between the parameterization of the two schemes leads to different patterns of sensitivities.

Unlike previous studies, predictive capabilities of these schemes are investigated in the configuration of one-dimensional laminar premixed flames without fixed temperature profiles. This work is partly motivated by the search for suitable schemes for subsequent simulations of DME combustion employing detailed chemical kinetics but in complex fluid flow regimes. In order to limit the complexity of this study, more recent updates of DME oxidation mechanisms [8] or thermal decomposition pathways [12] as well as the reduced scheme proposed by Chin et al. [13] were not taken into account.

Based on previous findings (e.g. [2,14]), it is expected that the overall uncertainty of key predictive targets of the chemical kinetic model at the given conditions will be driven by only a few parameters. Screening methods based on local sensitivity analysis were therefore developed to improve the efficiency of the subsequent QRS-HDMR approach. A further goal was to develop an intuitive interface for sensitivity analysis based on implementation of open-source software tools, thus supporting the wider applicability of the QRS-HDMR method for future studies related to the combustion community. Thus, an important objective of this work is to perform a pilot case study aimed at testing and further improving the specific-purpose software tools.

Methodology and implementation

The Cantera software toolbox (version 2.0.0) [15] was employed for modeling the structure of the one-dimensional premixed flat flames. As discussed in [2,16,17], global sensitivity analysis is based on quasi-random sampling of the model input parameters and hence a large number of model simulations should be performed for samples of input parameters which fall within the uncertainty boundaries of the input space. This process requires automation and hence the original C++ kernel of the Cantera code was interfaced via specific-purpose Python scripts designed to perform automatically appropriate calculations for the global sensitivity study. Implementation through such scripts enables the progress of multiple simulations and data manipulation in an efficient way on an arbitrary (Windows/Unix) computational platform. Additional subroutines and libraries were developed or linked (e.g. [18] used for generating the Sobol' quasi-random sequence, see later) in order to provide the simulation results in the required data format for the global sensitivity study. The routines were designed to be general enough to be applied to a wide variety of combustion schemes and configurations.

Available chemical kinetic schemes were modified according to requirements of our study. Data conversion from CHEMKIN format to Cantera input format (to *.cti files including chemical kinetic, thermodynamic and transport properties) was first performed. Forward and reverse reactions are specified separately in the

original LLNL scheme published by Fischer et al. [4], therefore, reaction rate constants were converted to reversible form. Further modification of this scheme was achieved by omitting some minor redundant species in accordance with [9]. The modified scheme included 231 reversible reactions and 44 species. In the case of the "Princeton" scheme, appropriate reaction rate constants for atmospheric pressure and nitrogen as a batch gas were specified. The final scheme consisted of 285 reactions and 53 species after the elimination of reactions with helium and argon atoms.

A mixture-averaged transport model was assumed to be sufficient for the given level of global sensitivity analysis. Numerical simulations with multicomponent transport considerably increased the computational cost and for the non-stoichiometric DME/air mixtures studied here, the application of multicomponent transport has only a minor effect on the modeling results, as reported for predictions of laminar flame speed by Wang et al. [8]. Radiative heat transfer as well as the effect of buoyancy forces was neglected throughout this study. A minimum of 100 non-uniformly spaced grid points were used to cover the computational domain of length $z = 5$ mm. Appropriate tolerance criteria and levels of grid refinement were selected to ensure sufficiently precise and robust converged steady-state solutions for each scheme. Computational times for the simulation of each flame were of the order of several minutes on a single processor. Since quite wide regions of parameter space were explored there were a number of unsuccessful simulations which did not achieve convergence at prolonged computational times (ten times the average computational time). Approximately 1% of the total number of samples N_S were excluded for this reason except in the case of fuel-lean conditions for both schemes, where the number of excluded samples was nearly 10%.

Prior to the global sensitivity and uncertainty analysis, identification of the most important reactions was performed using a screening method based on local sensitivities. Flame temperature maxima (T_{\max}), and peak methane ($X_{\text{CH}_4, \max}$) and formaldehyde ($X_{\text{CH}_2\text{O}, \max}$) concentrations were chosen as appropriate target quantities in this study. Different factors ranging from 1.1 to 1.5 (10% to 50% increase) for multiplication of the A -factor for the reaction rate were applied within the framework of local sensitivity analysis. Case-specific threshold levels were set, below which reactions were deemed to exhibit low enough sensitivity to be excluded from the subsequent global study. Four sets of important reactions, each containing about twenty A -factors, were obtained separately for fuel-lean and fuel-rich conditions for the two chemical schemes.

The assignment of uncertainty factors to individual reaction rates is the key first step for global sensitivity analysis. Therefore, Arrhenius plots were studied for each of the selected reactions in order to explore the agreement of nominal reaction rate expressions proposed by [4] and [11] with reviewed data having the

uncertainty factors properly assigned (e.g. [19]). The entire space over which the pre-exponential factors A_i (where i is the number of selected reactions) should be varied within the framework of global sensitivity analysis in most case exceeds the multiplication factor used for estimating the local sensitivities. However, only in extremely non-linear cases would a reaction with very low linear sensitivity exhibit a very high global one and hence the screening method is assumed to be useful for this pre-selection of reactions in order to reduce the dimension of the sampling space within the global study. Uncertainty factors (G_i) for all reactions were determined based on the values estimated from published reviews of data (e.g. [19], available from <http://kinetics.nist.gov>). Additionally, Arrhenius plots were constructed if the reaction rate constants for the given scheme differed from the reviewed values. In the case of significant differences (within the temperature range of 300 K to 2000 K) the uncertainty factor proposed in the literature was increased to capture this fact.

HDMR provides an efficient response surface generation method well suited for calculating the variance based sensitivity indices. Application of the QRS technique enables uniform coverage of the entire (i -dimensional) input space within the uncertainty limits set. A Sobol' sequence [20] was used for the sampling strategy and flame calculations performed for each selected sample. The MATLAB based software tool GUI-HDMR [16] was then used to fit an HDMR to the input-output response surface for the target quantities (T_{max} , $X_{CH4,max}$, $X_{CH2O,max}$) and global sensitivity indices were determined with respect to the selected A -factors.

Results and Discussion

Firstly, initial simulation of flame profiles were performed for lean and rich flames using the selected schemes and compared to experimental data. Reasonable agreement was found between the absolute values of T_{max} in the post-combustion region. In all cases except the "Princeton" scheme at fuel rich conditions, the results of simulations predict the experimental T_{max} within the experimental error (± 40 K) reported in [10].

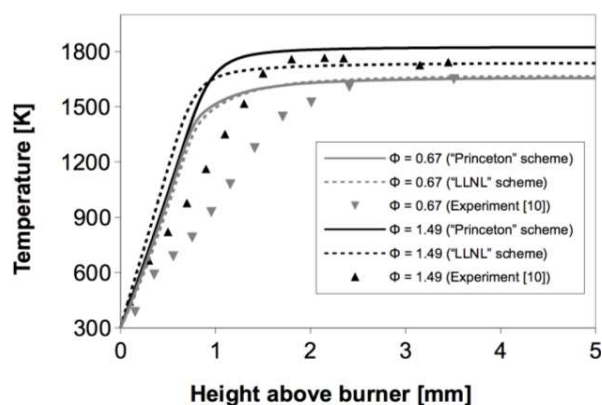


Figure 1. Temperature profiles for the two schemes studied for rich and lean atmospheric flames.

Temperature profiles depicted in Figure 1 show much narrower reaction zones predicted by the numerical simulations compared to experimental data. Such disagreement can be caused by different boundary conditions considered in the model. In the model, the temperature is not set as a fixed profile, but is iteratively solved together with the species profiles. The inlet mass flux of the DME/air mixture is determined by the fuel and air velocities provided by [10] assuming a top hat profile over the entire surface of the McKenna flat flame burner. Other hydrodynamic circumstances of the experimental setup (e.g. burner surrounding or flue gas outlet conditions) can also play an important role here. Similar effects were also observed in predicted concentrations of methane and formaldehyde. However, the relative positions of temperature and concentration maxima were not considered by the following study, where only the maxima of the target quantities were determined and further analyzed.

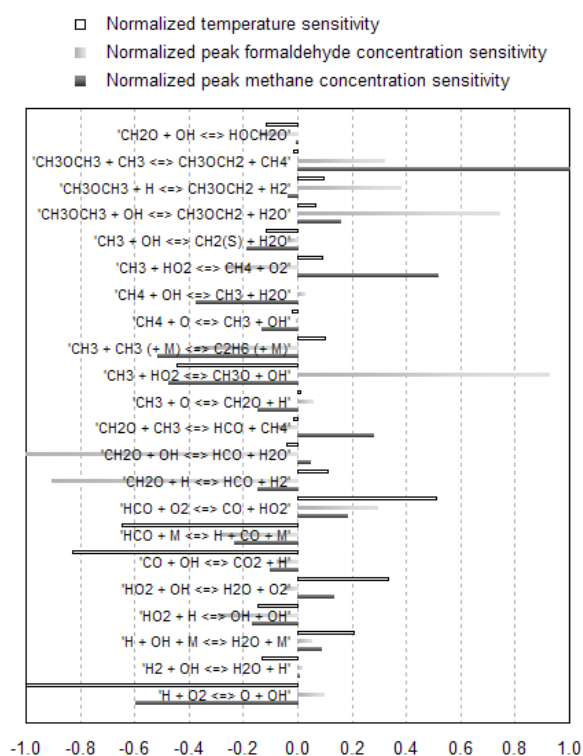


Figure 2. Normalized local sensitivities for selected target outputs for flames simulated using the "Princeton" scheme with $\Phi = 0.67$.

Local normalized sensitivities of selected reactions for the "Princeton" scheme at $\Phi = 0.67$ showing the impact of 50% increases to A -factors on target quantities are shown in Fig. 2. Further local sensitivity analysis was performed for fuel-rich and fuel-lean conditions. In each case, a set of reactions for the global sensitivity analysis was selected based on the following threshold criteria $abs(\Delta T_{max})/T_{max} > 0.2\%$ or $abs(\Delta X)/X > 2\%$. This strategy could be proposed as appropriate screening method for further studies concerning global

sensitivity and uncertainty of detailed chemical kinetic models of DME oxidation in laminar flames. Nevertheless, a more detailed benchmark study compared to other screening strategies (e.g. the Morris method [21]) would be required to assess the broader applicability of this approach.

A total sample size of $N_S = 1024$ was initially selected for the QRS-HDMR study according to previous experience for 1-D flame simulations [17]. This was sufficient for fitting species concentration data. Nevertheless, in order to obtain an accurate HDMR meta-model (to achieve coefficient of determination $R^2 > 95\%$) for temperature predictions, it was necessary increase N_S to 2048.

For the quasi-random samples obtained it is possible to construct a probability density distribution (*pdf*) for each of the target outputs (space limitations prevent us from showing them here). For T_{max} , the 2σ values from the *pdf* are within 20% of the mean predicted values and therefore the schemes could be considered to be fairly robust for the prediction of peak temperatures. For $X_{CH_4,max}$ and $X_{CH_2O,max}$ wider distributions are obtained with 2σ differing from the mean values of the *pdf* by more than a factor of 2 in some cases. The maximum concentrations of these minor combustion products therefore appear to be predicted with less certainty than the peak temperature. The sources of this uncertainty were explored via the global sensitivity coefficients.

Due to space limitations, demonstrative examples of the global sensitivity analysis are presented here via summary tables of the first-order sensitivity indices S_i . The highest ranked first-order sensitivities for T_{max} are reasonably consistent between both of the schemes tested (Table 1). The reason is that the highest ranked reactions $H+O_2$, $HCO (+M)$, $CO+OH$ and CH_3+HO_2 have fairly similar parameterizations within both schemes across a wide temperature range as demonstrated in Table 4. The temperature predictions

for both the lean and rich flames appear therefore to be reasonably robust as supported by the agreement between the schemes shown in Figure 1.

For $X_{CH_4,max}$ there is some disagreement between the ranking of the key reactions highlighted by the global sensitivity analysis (Table 2). For both flames the reaction $CH_3OCH_3+CH_3$ shows the dominant sensitivity for the ‘‘Princeton’’ scheme whilst $CH_3+CH_3 (+M)$ does for the ‘‘LLNL’’ scheme. There are clear differences between the adopted rates for $CH_3OCH_3+CH_3$ between the two schemes which reach a factor of 3 at high temperatures (see Table 4). The reaction rate for $CH_3OCH_3+CH_3$ in the case of the ‘‘LLNL’’ scheme is reported [4] to be based on the best-fit to available experimental and theoretical data. Further discussion on this reaction concerning the increased rate constant at higher temperature adopted for the ‘‘Princeton’’ scheme is provided by Zhao et al. [11]. However, it was emphasized that rigorous investigation of the rate of this reaction at temperatures above 900 K is required. The difference between estimated rates for the two schemes studied here leads to very different sensitivities to this reaction for $X_{CH_2O,max}$ in the rich flame. This reveals that better quantification of this reaction rate would significantly help to improve the prediction of minor products within DME/air flames.

The importance of $HCO (+M)$ and CH_3+HO_2 reactions was highlighted within the sensitivity analysis performed by previous investigators [4,6-9,11]. In contrast to these previous studies, due to relatively high input uncertainties related to these reactions, their sensitivities were observed in this global study to be of comparable magnitude to the dominant reactions identified by local sensitivity analysis ($CO+OH \leftrightarrow CO_2+H$ and $H+O_2 \leftrightarrow O+OH$). This stresses the importance of taking input uncertainties into account within sensitivity studies as highlighted in [22].

Table 1. First order sensitivities S_i , G_i and importance ranking of each reaction for output T_{max} .

Fuel-lean ($\Phi = 0.67$)	‘‘Princeton’’ scheme			‘‘LLNL’’ scheme		
	Reaction	G_i	S_i	Rank	G_i	S_i
HCO + M \leftrightarrow H + CO + M	10	0.385	(1)	10	0.379	(1)
CO + OH \leftrightarrow CO ₂ + H	3.16	0.261	(2)	3.16	0.293	(2)
CH ₃ + HO ₂ \leftrightarrow CH ₃ O + OH	10	0.211	(3)	10	0.100	(4)
H + O ₂ \leftrightarrow O + OH	1.65	0.074	(4)	3	0.285	(3)
CH ₂ O + OH \leftrightarrow HOCH ₂ O	10	0.025	(5)	10	-	-
CH ₃ + OH \leftrightarrow CH ₂ (S) + H ₂ O	10	0.010	(9)	10	0.014	(5)
Fuel-rich ($\Phi = 1.49$)	‘‘Princeton’’ scheme			‘‘LLNL’’ scheme		
Reaction	G_i	S_i	Rank	G_i	S_i	Rank
H + O ₂ \leftrightarrow O + OH	1.65	0.246	(1)	3	0.566	(1)
CH ₃ + HO ₂ \leftrightarrow CH ₃ O + OH	10	0.239	(2)	10	0.059	(3)
HCO + M \leftrightarrow H + CO + M	10	0.159	(3)	10	0.254	(2)
CH ₃ + H (+M) \leftrightarrow CH ₄ (+M)	10	0.124	(4)	-	-	-
CH ₃ OCH ₃ \leftrightarrow CH ₃ + CH ₃ O	10	0.021	(5)	10	0.019	(5)
CH ₃ + OH \leftrightarrow CH ₂ O + H ₂	-	-	-	10	0.025	(4)

Table 2. First order sensitivities S_i , G_i and importance ranking of each reaction for output $X_{CH_4,max}$.

Fuel-lean ($\Phi = 0.67$)	"Princeton" scheme			"LLNL" scheme			
	Reaction	G_i	S_i	Rank	G_i	S_i	Rank
	$CH_3OCH_3 + CH_3 \leftrightarrow CH_3OCH_2 + CH_4$	10	0.469	(1)	10	0.145	(2)
	$CH_3 + HO_2 \leftrightarrow CH_3O + OH$	10	0.161	(2)	10	0.060	(6)
	$HCO (+ M) \leftrightarrow H + CO (+ M)$	10	0.045	(3)	10	0.060	(5)
	$CH_3 + HO_2 \leftrightarrow CH_4 + O_2$	5	0.039	(4)	5	0.077	(4)
	$CH_3 + CH_3 (+ M) \leftrightarrow C_2H_6 (+ M)$	3	0.035	(5)	10	0.229	(1)
	$CH_4 + OH \leftrightarrow CH_3 + H_2O$	2	0.008	(9)	10	0.128	(3)
Fuel-rich ($\Phi = 1.49$)	"Princeton" scheme			"LLNL" scheme			
Reaction	G_i	S_i	Rank	G_i	S_i	Rank	
	$CH_3OCH_3 + CH_3 \leftrightarrow CH_3OCH_2 + CH_4$	10	0.540	(1)	10	0.102	(3)
	$CH_3 + HO_2 \leftrightarrow CH_3O + OH$	10	0.139	(2)	10	0.052	(5)
	$HCO (+ M) \leftrightarrow H + CO (+ M)$	10	0.071	(3)	10	0.217	(2)
	$CH_3 + CH_3 (+ M) \leftrightarrow C_2H_6 (+ M)$	3	0.065	(4)	10	0.366	(1)
	$CH_3 + H (+ M) \leftrightarrow CH_4 (+ M)$	10	0.030	(5)	-	-	-
	$H + O_2 \leftrightarrow O + OH$	1.65	0.018	(6)	3	0.060	(4)

Table 3. First order sensitivities S_i , G_i and importance ranking of each reaction for output $X_{CH_2O,max}$.

Fuel-lean ($\Phi = 0.67$)	"Princeton" scheme			"LLNL" scheme			
	Reaction	G_i	S_i	Rank	G_i	S_i	Rank
	$CH_2O + OH \leftrightarrow HCO + H_2O$	10	0.286	(1)	10	0.357	(1)
	$CH_3OCH_3 + OH \leftrightarrow CH_3OCH_2 + H_2O$	10	0.198	(2)	10	0.207	(2)
	$CH_3 + HO_2 \leftrightarrow CH_3O + OH$	10	0.119	(3)	10	0.073	(4)
	$CH_2O + H \leftrightarrow HCO + H_2$	3	0.074	(4)	3	0.105	(3)
	$CH_3OCH_3 + H \leftrightarrow CH_3OCH_2 + H_2$	10	0.066	(5)	10	0.070	(5)
Fuel-rich ($\Phi = 1.49$)	"Princeton" scheme			"LLNL" scheme			
Reaction	G_i	S_i	Rank	G_i	S_i	Rank	
	$CH_3OCH_3 + CH_3 \leftrightarrow CH_3OCH_2 + CH_4$	10	0.251	(1)	10	0.032	(6)
	$CH_2O + H \leftrightarrow HCO + H_2$	3	0.207	(2)	3	0.299	(1)
	$CH_3OCH_3 + H \leftrightarrow CH_3OCH_2 + H_2$	10	0.170	(3)	10	0.282	(2)
	$HCO (+ M) \leftrightarrow H + CO (+ M)$	10	0.110	(4)	10	0.095	(3)
	$CH_2O + OH \leftrightarrow HCO + H_2O$	10	0.084	(5)	10	0.086	(4)
	$CH_3OCH_3 + OH \leftrightarrow CH_3OCH_2 + H_2O$	10	0.041	(6)	10	0.050	(5)

Moreover, in the case of CH_3+HO_2 two competing reaction channels (termination step leading to CH_4 and O_2 and propagation step forming CH_3O and OH radicals) are identified to be of critical importance for predicting the methane concentrations for fuel-lean conditions.

Uncertainties in the prediction of formaldehyde are also influenced by uncertainties in the A -factors for CH_2O consumption reactions (by hydrogen abstraction by OH radicals or H atoms). The adopted rates for these reactions are consistent between the schemes but in total they can contribute up to 40% of the total uncertainty in predicted peak CH_2O within the rich flame.

Conclusions

Based on the present study the most important reactions in premixed flat flames of fuel-rich and fuel-lean DME/air mixture were identified and their global sensitivity indices were determined. This system provides a representative example demonstrating the influence of uncertainties within chemical kinetic schemes in the context of predicting minor products from combustion processes. Initial estimates of the potential range of errors associated with prediction of peak temperatures and concentrations of important species within premixed flames of oxygenated fuel was provided.

Table 4. Comparison of forward rate constants (in $\text{cm}^3\text{mol}^{-1}\text{s}^{-1}$) for the two schemes at selected temperatures.

Reaction	"Princeton" scheme			"LLNL" scheme		
	$k_{f,750\text{K}}$	$k_{f,1000\text{K}}$	$k_{f,1500\text{K}}$	$k_{f,750\text{K}}$	$k_{f,1000\text{K}}$	$k_{f,1500\text{K}}$
$\text{HCO} + \text{M} \leftrightarrow \text{H} + \text{CO} + \text{M}$	1.73×10^9	2.53×10^{10}	4.00×10^{11}	2.76×10^9	3.58×10^{10}	4.14×10^{11}
$\text{CO} + \text{OH} \leftrightarrow \text{CO}_2 + \text{H}$	1.32×10^{11}	1.87×10^{11}	3.31×10^{11}	1.40×10^{11}	1.95×10^{11}	3.43×10^{11}
$\text{CH}_3 + \text{HO}_2 \leftrightarrow \text{CH}_3\text{O} + \text{OH}$	1.76×10^{13}	1.48×10^{13}	1.36×10^{13}	1.10×10^{13}	1.10×10^{13}	1.10×10^{13}
$\text{H} + \text{O}_2 \leftrightarrow \text{O} + \text{OH}$	3.51×10^9	5.06×10^{10}	6.95×10^{11}	2.98×10^9	4.78×10^{10}	7.67×10^{11}
$\text{CH}_3\text{OCH}_3 + \text{CH}_3 \leftrightarrow \text{CH}_3\text{OCH}_2 + \text{CH}_4$	3.04×10^9	4.54×10^{10}	1.06×10^{12}	9.40×10^8	1.27×10^{10}	3.38×10^{11}
$\text{CH}_3 + \text{CH}_3 (+\text{M}) \leftrightarrow \text{C}_2\text{H}_6 (+\text{M})$	2.10×10^{13}	1.77×10^{13}	1.38×10^{13}	2.60×10^{13}	2.07×10^{13}	1.43×10^{13}
$\text{CH}_4 + \text{OH} \leftrightarrow \text{CH}_3 + \text{H}_2\text{O}$	4.20×10^{11}	1.15×10^{12}	3.96×10^{12}	3.73×10^{11}	1.06×10^{12}	3.99×10^{12}
$\text{CH}_2\text{O} + \text{OH} \leftrightarrow \text{HCO} + \text{H}_2\text{O}$	1.14×10^{13}	1.49×10^{13}	2.23×10^{13}	1.14×10^{13}	1.49×10^{13}	2.23×10^{13}
$\text{CH}_3\text{OCH}_3 + \text{OH} \leftrightarrow \text{CH}_3\text{OCH}_2 + \text{H}_2\text{O}$	5.76×10^{12}	9.21×10^{12}	1.86×10^{13}	6.05×10^{12}	1.03×10^{13}	2.28×10^{13}
$\text{CH}_2\text{O} + \text{H} \leftrightarrow \text{HCO} + \text{H}_2$	2.63×10^{12}	7.21×10^{12}	2.47×10^{13}	2.60×10^{12}	6.60×10^{12}	2.00×10^{13}
$\text{CH}_3\text{OCH}_3 + \text{H} \leftrightarrow \text{CH}_3\text{OCH}_2 + \text{H}_2$	1.12×10^{12}	3.90×10^{12}	1.73×10^{13}	8.14×10^{11}	2.62×10^{12}	1.08×10^{13}

Ongoing activities focused on different target quantities (e.g. laminar flame speed) or non-premixed counter-flow flames involving multi-component transport will in future work supplement the findings obtained by the global sensitivity analysis reported here.

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