

# Uncertainty Analysis Backed Development of Combustion Mechanisms

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## Abstract

Uncertainty analysis was used to back the development of H<sub>2</sub>/air and wet CO/air combustion mechanisms. The Leeds Methane Oxidation Mechanism was updated on the basis of the latest literature data. Uncertainties of the simulation results, caused by the uncertainties of the kinetic parameters and the heat of formation data, were analysed. The methods used were local uncertainty analysis and Monte Carlo Analysis with Latin Hypercube Sampling. There was always satisfactory agreement between the simulation results and the bulk experimental data, but in some cases the uncertainties of the simulation results were large.

## Introduction

Development of detailed combustion mechanisms is always based on the utilization of direct experimental data for the elementary reactions. Experimental data for species, *e.g.* thermodynamic data, are also used in combustion models. Then, applicability of the developed combustion mechanism is tested against bulk experimental data. The simulations provide the output of the model at the finally selected parameter set only and do not reveal the uncertainty of the simulation results. However, comparison of the experimental and simulation uncertainties is very important for the development of reaction mechanisms that are needed to be accurate in a wide range of conditions. Uncertainty analysis reveals which results are well supported by the model and which ones are merely nominal values that were obtained using the selected set of input parameters.

In combustion kinetics, Warnatz was the first [1] who considered the uncertainty of kinetic parameters. His 'sensitivity-uncertainty indices' were based on the uncertainty of kinetic parameters and the local sensitivity coefficients, and provided an unbiased order of reactions that caused the highest uncertainty of simulation results. These indices, however, do not characterize the uncertainty of simulation results. Bromly *et al.* [2] carried out a local joint kinetic and thermodynamic uncertainty analysis of a model of the low-temperature NO-sensitised oxidation of methane. The 'impact factors' of Bromly *et al.* had features similar to the Warnatz' indices. Brown and his co-workers [3] estimated the variance of the calculated hydrogen-air flame velocity from the uncertainties of the kinetic parameters. All these methods for the uncertainty analysis of combustion models were compared and discussed by Turányi *et al.* [4]. The article of Turányi *et al.* [4] also included an algorithmic description of the calculation of the variance of simulation results of chemical kinetic

models from the uncertainties of kinetic and thermodynamic parameters, using the local uncertainty analysis approach. Not only this local method, but global uncertainty analysis was also applied here.

## Reaction mechanisms and simulation codes

The Leeds methane oxidation mechanism [5] provided the basis for the further development of the H<sub>2</sub>/air and wet CO/air combustion mechanisms. The hydrogen oxidation mechanism is naturally separated from the other parts of the methane oxidation mechanism because the corresponding species do not contain carbon. The species considered in the hydrogen-air combustion mechanism were H<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>, H, O, OH, HO<sub>2</sub>, N<sub>2</sub>, and Ar. The wet CO oxidation mechanism consisted of all the above species and also included CO, CO<sub>2</sub>, and HCO. Accordingly, the wet CO oxidation mechanism incorporated the whole hydrogen oxidation mechanism and also included the reactions of the carbon-atom species above.

The rate parameters of all reactions were revised using the latest CEC evaluation [6]. All new recommendations were accepted, except for that of reaction O<sub>2</sub>+H=OH+O. The new recommended value is ten times smaller than the previous one [7] and using the new value the bulk experiential data could not be reproduced. In all the simulations presented here the preexponential factor of this reaction was taken to be 0.88 times of the latest CEC evaluation value [6]. The enthalpies of formation of species were updated according to a recent review, published in article [4]. Uncertainty factors *f* of the rate parameters were taken from data evaluations (mainly from [7]). The uncertainty factors were converted to the variances of rate coefficients using the method described in [4]. The assumed variances of enthalpies of formation were identical to those of article [4].

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The calculations were carried out with the CHEMKIN-II package [8]. Programs SENKIN [9] and PREMIX [10] were modified for carrying out sequential calculations with many altered parameter sets required by the global uncertainty analysis methods. Local and global uncertainty analyses were carried out with purpose written Fortran codes.

### Local uncertainty analysis

Sensitivity analysis is the common name for a family of tools for investigating the relations between the input parameters and output values of mathematical models [11]. Local sensitivity analysis is widely used in chemical kinetics to explore and understand complex reaction mechanisms (see, *e.g.* [12] and [13]). Local sensitivity coefficients are the partial derivatives of the output values with respect to the input parameters. Using the rules of error propagation, the contribution of the uncertainty of kinetic parameter  $k_j$  to the uncertainty of modelling result  $Y_i$  can be calculated:

$$\sigma_{K_j}^2(Y_i) = \left( \partial Y_i / \partial \ln k_j \right)^2 \sigma^2(\ln k_j),$$

where  $\sigma^2(\ln k_j)$  is the variance of the logarithm of rate coefficient  $k_j$  and  $\partial Y_i / \partial \ln k_j$  is the semi-normalized sensitivity coefficient. The contributions of the uncertainties of enthalpies of formation can be calculated in a similar way:

$$\sigma_{T_j}^2(Y_i) = \left( \partial Y_i / \partial \Delta_f H_{298}^\circ(j) \right)^2 \sigma^2(\Delta_f H_{298}^\circ(j)).$$

The sum of the contributions of kinetic and thermodynamic uncertainties provide the variance of modelling result  $Y_i$ :

$$\sigma^2(Y_i) = \sum_j \sigma_{K_j}^2(Y_i) + \sum_j \sigma_{T_j}^2(Y_i)$$

The percentage share  $S\%_{ij}$  is a good indication of the contribution of the partial variance of kinetic or thermodynamic parameter  $j$  to variance  $\sigma^2(Y_i)$ :

$$S\%_{ij} = \frac{\sigma_j^2(Y_i)}{\sigma^2(Y_i)} \times 100$$

The calculated variances are exact for linear models and are estimates only for highly non-linear chemical kinetic models. However, our experience is that these local estimates are not far from the corresponding more precise values, determined by the methods of global uncertainty analysis.

### Monte Carlo Analysis with Latin Hypercube Sampling (LHS MC)

Monte Carlo (MC) simulations have become increasingly common in atmospheric kinetics for global uncertainty analysis. Monte Carlo analysis [11] includes that large number of parameter sets are generated according to the probability density functions of these parameters. Then, the model is simulated with each of these parameter sets and the results are processed with statistical methods. The cornerstone of this approach is the application of an

efficient and unbiased method for the selection of the parameter sets.

Using the method of Latin Hypercube Sampling [11], the range of parameters to be varied during the MC simulations is divided into intervals of equal probability. The parameter values are then randomly sampled, independently in each interval and the selected values of the parameters are randomly grouped. This ensures that the parameter space is represented with a good approximation of full coverage. In the Monte Carlo calculations presented in this paper, the models were simulated with 1000 parameter sets. The analysis of the MC simulation results included the calculation of the means and the variances of the model output. This way, quantitative uncertainties of the calculated concentrations could be obtained at several time points.

### Uncertainties of hydrogen combustion models

Laminar flame velocity of hydrogen/air mixtures at atmospheric pressure was simulated in a wide range of equivalence ratio. The simulation results were compared with recent experimental data [14-17].

The measured laminar flame velocity values of lean mixtures were in good agreement with each other and with the simulation results. Interestingly, the calculated modelling uncertainty was also small in this region. For moderately rich and rich mixtures, there was systematic deviation between the experimental results of Dowdy *et al.* [16] and of Aung *et al.* [17]. Our simulation results were closer to the data of Dowdy *et al.*, but the LHS MC uncertainty analysis revealed that the data of Aung *et al.* were also within the range of uncertainty. Figure 1 shows the calculated laminar flame velocity as a

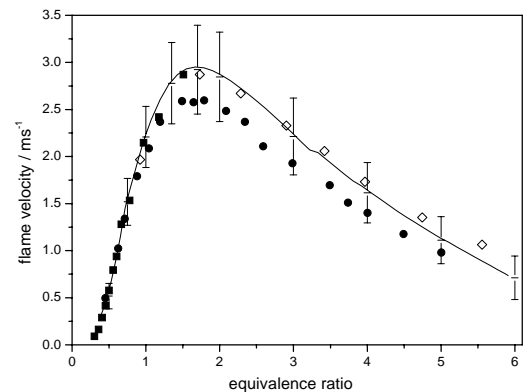


Fig. 1. Flame velocity as a function of equivalence ratio in hydrogen/air mixtures. The solid line is the simulation result and the vertical intervals represent the  $2\sigma$  uncertainty of simulation results due to the uncertainty of kinetic and thermodynamic data. The dots refer to the experimental data: ■ - Law *et al.* [14, 15] ◇ - Dowdy *et al.* [16] ● - Aung *et al.* [17].

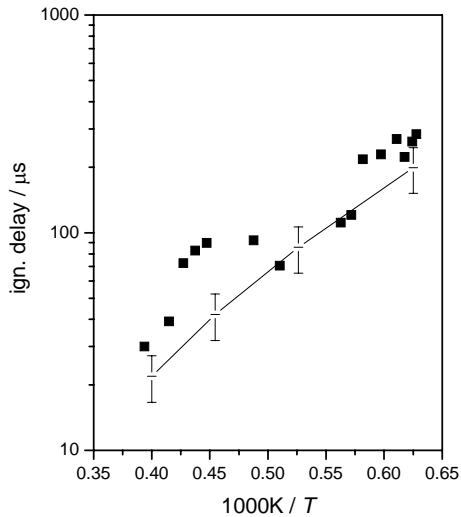


Fig. 2. Ignition delays in 1% H<sub>2</sub>, 1% O<sub>2</sub>, 98% Ar mixtures as a function of initial temperature. The solid line is the simulation result, the vertical intervals represent the 2 $\sigma$  uncertainty of simulation results, and the dots refer to the experimental data of Asaba *et al.* [18].

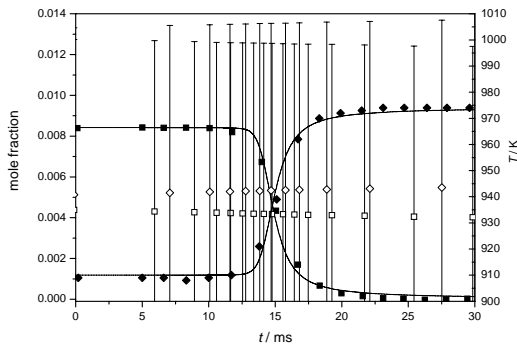


Fig. 3. Temperature and H<sub>2</sub> concentration profiles during the combustion of a lean H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> mixture at 1 atm. The solid line is the simulation result, the vertical intervals represent the 2 $\sigma$  uncertainty of simulation results, the empty symbols correspond to the average of the MC simulation results, and the dots refer to the experimental data of Yetter *et al.* [19].

function of equivalence ratio, the 2 $\sigma$  uncertainty of simulation results calculated by Monte Carlo Analysis with Latin Hypercube Sampling, and the experimental data.

Figure 2 shows the comparison between the experimental [18] and the simulated ignition delay times in a 1% hydrogen, 1% oxygen, 98% argon mixture as a function of initial temperature. In these experiments, there was no sharp increase of temperature and the ‘ignition delay’ was defined by the time when the concentration of OH reached

$1 \times 10^{-8}$  mol dm<sup>-3</sup>. This Figure shows that the temperature dependence of the simulated and the experimental ignition delays were similar, and also the simulated and experimental uncertainties were of similar magnitude. The calculated ignition delays were slightly shorter than the experimental ones and the simulated and experimental uncertainty regions did not overlap perfectly.

Yetter, Dryer and Rabitz [19] measured the temperature and the concentration profiles of H<sub>2</sub>, O<sub>2</sub>, and H<sub>2</sub>O in a flow reactor at 1 atm using a 0.842% H<sub>2</sub>, 1.52% O<sub>2</sub> and 97.638% N<sub>2</sub> mixture. The results are shown in Figure 3. The calculated nominal values are very accurate, but the modelling uncertainties are very large. This means that small changes of the values of the rate parameters, well within their ranges of uncertainty results in very different simulation results. Therefore, the good agreement of the simulation and experimental results does not mean that the system is well characterized by the model.

### Uncertainties of wet CO combustion models

Laminar flame velocity of atmospheric (95% carbon monoxide + 5% hydrogen) / air mixture was simulated in equivalence ratio range  $\phi = 0.5$ –6.0. Figure 4 shows the simulated flame velocity as a function of equivalence ratio, the 2 $\sigma$  uncertainty of it calculated by the LHS Monte Carlo Method and the experimental data of McLean *et al.* [20]. The simulated values were in good agreement with the experimental data, but the uncertainty ranges were larger than those of the hydrogen-air flame.

Local uncertainty analysis was used to investigate further this laminar wet CO flame. Table 1 contains the calculated value of laminar flame velocity, maximum temperature, and maximum concentrations of H, O, and OH at equivalence ratios  $\phi=0.5, 1.0, 2.0,$  and 4.0. The table also contains the 1 $\sigma$  uncertainty of these values and the uncertainty as the percentage of the nominal value. These figures are in good agreement (usually within 10%) with the LHS MC results.

In accordance with the previous methane flame uncertainty analysis results [4], the uncertainty of the calculated maximum flame temperature was found to be very small, especially in rich flames. The uncertainty of simulated flame velocity (3–10 cm s<sup>-1</sup>) is slightly higher than the typical measurement error. The uncertainties of the calculated maximum radical concentrations are surprisingly large, since these are usually in the range of 10–25%.

Table 2 provides the percentage share ( $S\%_{ij}$ ) of the variance of a kinetic or thermodynamic parameter to the variance of a simulation result. The table shows that the uncertainty of the rate parameters of reaction CO+OH=CO<sub>2</sub>+H is responsible for the high uncertainty of the laminar flame velocity ( $v_L$ ) and of the maximum concentrations of H, O, and OH at each investigated equivalence ratio.

Table 1

Calculated values,  $1\sigma$  uncertainty and percentage of the  $1\sigma$  uncertainty of laminar flame velocity ( $v_L$ /  $\text{cm s}^{-1}$ ), maximum temperature ( $T_{\max}$ /K), and maximum concentrations of H, O, and OH ( $\text{c/mole cm}^{-3}$ ) at equivalence ratios  $\phi=0.5, 1.0, 2.0,$  and  $4.0$  of freely propagating laminar flames of (95%  $\text{CO}+5\% \text{H}_2$ )/air mixtures.

$\phi$	0.5			1.0			2.0			4.0		
	value	$\sigma$	%	value	$\sigma$	%	value	$\sigma$	% $_{o_i}$	value	$\sigma$	%
$v_L$	10.778	2.672	24.79%	36.419	6.596	18.11%	62.606	10.313	16.47%	49.068	7.830	15.96%
$T_{\max}$	1751.569	6.497	0.37%	2382.165	2.947	0.12%	2163.142	1.314	0.06%	1631.417	1.079	0.07%
$c_H$	5.42E-09	2.89E-09	53.33%	3.95E-08	9.03E-09	22.89%	9.92E-08	1.52E-08	15.28%	8.98E-08	1.45E-08	16.10%
$c_O$	3.20E-08	1.04E-08	32.58%	8.80E-08	1.35E-08	15.33%	7.87E-08	1.02E-08	12.96%	2.20E-08	5.03E-09	22.92%
$c_{OH}$	9.62E-09	1.21E-09	12.58%	2.31E-08	6.24E-10	2.69%	2.01E-08	5.86E-10	2.91%	5.27E-09	1.05E-09	19.96%

Table 2

Percentage share ( $S\%_{o_{ij}}$ ) of the partial variances of kinetic parameters of reactions and enthalpies of formation of species, calculated for the laminar flame velocity ( $v_L$ ), maximum temperature ( $T_{\max}$ ), and maximum concentrations of H, O, and OH, at the conditions described in the caption of Table 1.

$\phi$	0.5		1.0	
	parameter	$S\%_{o_{ij}}$	parameter	$S\%_{o_{ij}}$
$v_L$	CO+OH=CO2+H	81.01%	CO+OH=CO2+H	87.64%
	O2+H+M=HO2+M	16.21%	O2+H+M=HO2+M	7.41%
	OH+HO2=H2O+O2	0.79%	H+HO2=2OH	2.00%
	OH	0.63%	OH+HO2=H2O+O2	1.07%
$T_{\max}$	CO+OH=CO2+H	80.96%	CO+O+M=CO2+M	28.98%
	O2+H+M=HO2+M	13.83%	CO+OH=CO2+H	18.93%
	CO	1.61%	O2+H+M=HO2+M	18.86%
	CO2	0.94%	CO	17.79%
			CO2	10.36%
$c_H$	CO+OH=CO2+H	59.33%	CO+OH=CO2+H	68.48%
	O2+H+M=HO2+M	39.65%	O2+H+M=HO2+M	26.83%
	OH	0.43%	H+O+M=OH+M	1.80%
	OH+HO2=H2O+O2	0.14%	CO+O+M=CO2+M	1.37%
$c_O$	CO+OH=CO2+H	55.57%	CO+OH=CO2+H	68.10%
	O2+H+M=HO2+M	43.30%	O2+H+M=HO2+M	25.90%
	OH	0.34%	H+O+M=OH+M	2.24%
	O2+H=OH+O	0.32%	CO+O+M=CO2+M	1.72%
$c_{OH}$	CO+OH=CO2+H	51.09%	OH	65.46%
	O2+H+M=HO2+M	40.30%	CO+OH=CO2+H	22.75%
	OH	7.59%	O2+H+M=HO2+M	6.72%
	OH+HO2=H2O+O2	0.28%	CO	1.15%
$\phi$	2.0		4.0	
	parameter	$S\%_{o_{ij}}$	parameter	$S\%_{o_{ij}}$
$v_L$	CO+OH=CO2+H	85.54%	CO+OH=CO2+H	51.34%
	O2+H+M=HO2+M	4.40%	O2+H=OH+O	15.99%
	H+HO2=2OH	3.31%	HCO+M=H+CO+M	11.58%
	OH+HO2=H2O+O2	1.53%	H+HO2=2OH	7.90%
$T_{\max}$	CO	51.81%	CO	46.62%
	CO2	30.21%	CO2	26.41%
	CO+O+M=CO2+M	14.07%	CO+O+M=CO2+M	13.37%
	CO+OH=CO2+H	2.21%	O2+H=OH+O	7.57%
$c_H$	CO+OH=CO2+H	75.34%	CO+OH=CO2+H	45.13%
	O2+H+M=HO2+M	11.50%	HCO+M=H+CO+M	15.45%
	H+O+M=OH+M	4.31%	O2+H=OH+O	14.07%
	CO+O+M=CO2+M	3.27%	H+HCO=CO+H2	7.63%
$c_O$	CO+OH=CO2+H	67.28%	O2+H=OH+O	64.05%
	O2+H+M=HO2+M	11.36%	CO+OH=CO2+H	12.34%
	O2+H=OH+O	8.43%	HCO+M=H+CO+M	8.44%
	H+O+M=OH+M	5.43%	CO+O+M=CO2+M	4.29%
	CO+O+M=CO2+M	4.28%		
$c_{OH}$	OH	64.44%	CO+OH=CO2+H	47.81%
	CO+OH=CO2+H	22.27%	O2+H=OH+O	37.20%
	H+OH+M=H2O+M	4.02%	HCO+M=H+CO+M	3.42%
	CO+O+M=CO2+M	3.31%	H2+O=OH+H	3.14%

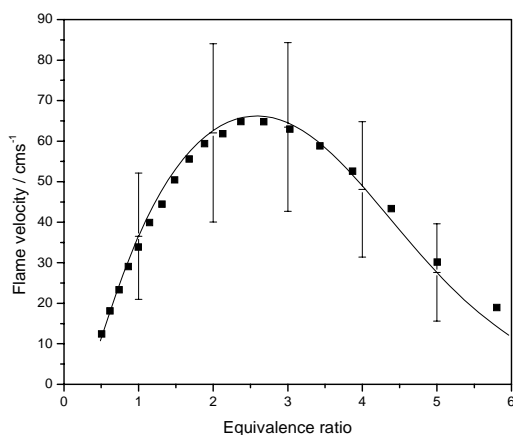


Fig. 4. Flame velocity as a function of equivalence ratio of (95% CO+5% H<sub>2</sub>)/air mixtures. The solid line is the simulation result, the vertical intervals represent 2 $\sigma$  uncertainty, and the dots refer to the experimental data of *McLean et al.* [20].

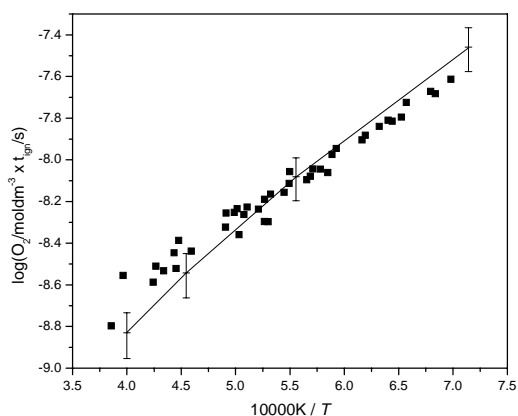


Fig. 5. Ignition delays in a 1% H<sub>2</sub>, 3% CO, 5% O<sub>2</sub>, 91% Ar mixture as a function of initial temperature. The solid line is the simulation result, the vertical intervals represent the 2 $\sigma$  uncertainty of simulation results, and the dots refer to the experimental data of *Gardiner et al.* [21].

Uncertainty of reactions  $O_2+H+M=HO_2+M$  and  $O_2+H=OH+O$  also cause high uncertainty to several model results. In very rich systems, the uncertainty of reaction  $HCO+M=H+CO+M$  also have some influence. In rich mixtures, the uncertainties of the enthalpy of formation of CO and CO<sub>2</sub> are the most responsible for the uncertainty of the maximum flame temperature, although this uncertainty is not significant. The uncertainty of the enthalpy of formation of OH highly influences the calculated OH concentration, except for in very rich mixtures. It is surprising, however, that most of the uncertainties of simulation results are caused by the uncertainties of only four rate parameters and a single enthalpy of formation.

Figure 5 compares the experimental [21] and the simulated ignition delay times in a 1% H<sub>2</sub>, 3% CO, 5% O<sub>2</sub>, 91% Ar mixture as a function of initial temperature. The temperature dependence of the simulated and the experimental ignition delays were similar, and also the simulated and experimental uncertainties were of similar magnitude, but there is a small systematic deviation between the two curves.

## Conclusions

Detailed combustion mechanisms are created using experimental data for the rate coefficients of elementary reactions and specific experimental data for the participating species. Predictions based on these mechanisms, like oxidation of the fuel at various conditions or pollutant formations, are tested by bulk experiments. In the cases of most proposed detailed reaction mechanisms, the agreement between the simulated and the experimental data was not bad, but also not perfect. Until now, there was not an objective basis to decide if the agreement had been satisfactory or not.

In this paper, the simulation results were always accompanied with uncertainty analysis results. Both local and global (Monte Carlo) uncertainty analyses were used. The method of local uncertainty analysis [4] allows fast calculation and provides information about the origin of uncertainty. This means that not only the variances of simulation results can be calculated, but also the contribution of the partial variances of kinetic and thermodynamic parameters to the overall variances of simulation results can be obtained. Local uncertainty analysis does not provide accurate uncertainties if these uncertainties are large or if the effects of the parameters are highly nonlinear. Monte Carlo analysis provides accurate uncertainties even in these cases, but the 'naïve' version of this method requires large number of simulations. The Latin Hypercube Sampling methodology offers an efficient Monte Carlo analysis, while the results remain unbiased.

The Leeds Methane Oxidation Mechanism was updated using the latest evaluated kinetic and thermodynamic data. The updated mechanism was tested against three hydrogen oxidation and two wet CO bulk experiments. The simulation results were always in good agreement with the experimental data. However, uncertainty analysis revealed that the 'good agreement' had different meaning in each case. The simulated flame velocity has relatively large uncertainty due to the uncertainties of the kinetic and thermodynamic data in both hydrogen-air and wet CO flames. There were no systematic deviations between the simulated and the experimental flame velocities. The experimental data were always within the range of uncertainty of the simulation results.

In case of ignition experiments, for both fuels the uncertainties of the simulated ignition delay times were small and comparable with the scatter of the experimental data. In both cases a small systematic

deviation was found between the simulated and the experimental values.

There was an almost perfect agreement between the temperature and concentration profiles of hydrogen oxidation, measured in a flow reactor by Yetter *et al.* and the simulated curves. However, the uncertainties of the calculated temperature and concentration profiles were found to be very large. This means that small modifications of the parameters, well within their range of uncertainty, provide very different results. Consequently, the current good agreement does not mean that the system is very well known.

Local uncertainty analysis of the wet CO flame revealed that uncertainties of the rate parameters of reactions  $\text{CO}+\text{OH}=\text{CO}_2+\text{H}$ ,  $\text{O}_2+\text{H}+\text{M}=\text{HO}_2+\text{M}$ ,  $\text{O}_2+\text{H}=\text{OH}+\text{O}$ , and  $\text{HCO}+\text{M}=\text{H}+\text{CO}+\text{M}$  cause high uncertainty to the calculated flame velocity, temperature, and the peak concentrations of radicals. The uncertainty of the enthalpy of formation of OH is highly responsible for the uncertainty of the calculated peak OH concentration.

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