

Optimisation of a hydrogen combustion mechanism

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Abstract

A large set of experimental data was collected for hydrogen combustion and used for the optimisation of a hydrogen combustion mechanism: ignition measurements in shock tubes (786 data points in 54 datasets) and rapid compression machines (166 data points in 9 datasets), and concentration–time profiles in jet-stirred reactors (152 data points in 9 datasets), covering wide ranges of temperature, pressure and equivalence ratio. The rate parameters to be optimised were determined by local sensitivity analysis at the conditions of the experiments. Using a global optimisation method, Arrhenius parameters of 8 reactions and the third body efficiency of Ar in the $\text{H} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$ reaction were determined. The obtained mechanism reproduces the experimental data better (including the flame velocity measurements; 631 data points in 71 datasets) than the other recent hydrogen combustion mechanisms.

Introduction

The reaction mechanism of hydrogen combustion is of central importance in combustion chemistry. Several new hydrogen combustion mechanisms were published in the last years; see *e.g.* the mechanisms of Ó Conaire *et al.* [1], Konnov [2], Hong *et al.* [3], Burke *et al.* [4], and Kéromnès *et al.* [5]. In all these mechanisms, most of the parameters were based on directly measured or theoretically calculated rate coefficient values, but also some of the rate parameters were tuned to improve the agreement with the results of indirect measurements, like ignition delay times or flame velocities. Although these mechanisms contain almost identical reaction steps and were developed by utilizing a similar set of experiments, the applied rate parameters and also the performances of the mechanisms at various experimental conditions are different.

In this work we applied a recently suggested method [6] to optimise a hydrogen combustion mechanism. Mechanism optimisation means that the rate parameters of several reaction steps are systematically changed within their uncertainty limits to give a better reproduction of the indirect experimental results. Several reaction mechanisms have been optimised by Frenklach *et al.* (see *e.g.* [7], [8]) and Wang *et al.* (see *e.g.* [9], [10]).

Encoding and processing of the experimental data

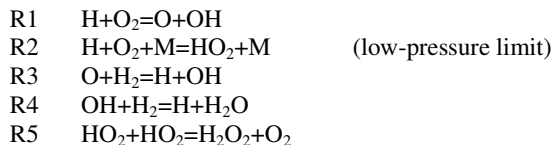
A large set of indirect experimental data was collected for hydrogen combustion: ignition measurements in shock tubes (786 data points in 54 datasets from 15 original publications) and rapid compression machines (166 data points in 9 datasets from one publication), flame velocity measurements (631 data points in 71 datasets from 20 publications) and concentration–time profiles in jet-stirred reactors (152 data points in 9 datasets from one publication). A dataset contains those data points that were measured on the same apparatus at the same time at similar

conditions except for one factor that was systematically varied. One experimental publication usually contains one or a few datasets. Our aim was to collect the results of all indirect measurements that were ever used for testing hydrogen combustion mechanisms and also all other data that have a similar quality and capability.

All indirect experimental data were encoded in PrIME file format [11], which is an XML scheme used for the systematic storage of various kinds of combustion experiments. Encoding the experimental conditions and results in PrIME format allows for an automatic simulation of all experiments. A MATLAB code was written that reads the PrIME data file and prepares the corresponding CHEMKIN-II [12] input files. The MATLAB code then starts the corresponding CHEMKIN simulation code (SENKIN, PREMIX or PSR), and collects the simulation results. The mechanism used in these calculations was the hydrogen combustion part of the recently elaborated mechanism of Kéromnès *et al.* [5]. The MATLAB code also carried out a local sensitivity analysis; for each simulated experimental data point the sensitivities of the simulation results with respect to the Arrhenius *A* parameters of the reaction steps and (if applicable) to the third body efficiencies were calculated.

Selection of rate parameters to be optimised

For each ignition delay time and jet-stirred reactor outlet concentration experimental point the top ten highest sensitivity parameters were selected. The analysis of these highly sensitivity parameters indicated that the rate parameters of the following reaction steps should be optimised:



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- R6 OH+OH+M=H₂O₂+M (low-pressure limit)
 R7 H₂O₂+H=H₂+HO₂
 R8 H+HO₂=H₂+O₂

This means that the rate parameters of these reactions can be determined from the available set of indirect experimental data. For each reaction step, the Arrhenius parameters A , n , E were optimised, except for reactions R2 and R5, where the temperature dependence could be described by Arrhenius parameters A and E . For reaction R2 and R6, the Arrhenius parameters refer to the low pressure limit. Also, the sensitivity analysis indicated that in reaction R2 the third body efficiency of Ar relative to N₂ can be determined.

Determination of the *a priori* uncertainty domain of the parameters

All parameter optimisation methods require the definition of the domain of uncertainty of the parameters, because the optimal parameter set is looked for within this domain. Parameter optimisation involving all Arrhenius parameters requires the knowledge of the joint domain of uncertainty of the Arrhenius parameters, but the chemical kinetics databases (like the NIST Chemical Kinetics Database [13]) and critical data evaluations (like those of Baulch *et al.* [14]) contain information only about the (possibly temperature-dependent) uncertainty of the rate coefficient k in the form of uncertainty parameter f :

$$f(T) = \log_{10}(k(T)/k^{\min}(T)) = \log_{10}(k^{\max}(T)/k^0(T))$$

where k^0 is the recommended value of the rate coefficient and values below k^{\min} and above k^{\max} are considered to be very improbable. Assuming that the minimum and maximum values of the rate coefficients correspond to 3σ deviations from the recommended values on a logarithmic scale, the uncertainty f can be converted [15] to the standard deviation of the logarithm of the rate coefficient at a given temperature T using the equation:

$$\sigma(\ln k) = \ln 10 \sigma(\log_{10} k) = \frac{\ln 10}{3} f(T)$$

Nagy and Turányi recently published ([16], [17]) a method that allows for the conversion of temperature dependent uncertainty parameter f to the covariance matrix the Arrhenius parameters. This covariance matrix defines the *a priori* domain of uncertainty of the rate parameters based on all direct measurements and theoretical calculations available in the literature, but without considering the results of optimisation.

The method of Nagy and Turányi requires the following steps for each investigated reaction:

(i) The mean Arrhenius expression of the rate coefficient is selected. This is usually identical to the values recommended in data evaluations or used in recently published mechanisms.

(ii) Arrhenius expressions for the rate coefficients, based on direct experimental determinations and high level theoretical calculations, are collected. These Arrhenius expressions are usually valid only in a narrow range of temperature.

(iii) The Arrhenius expressions above (*e.g.* see the dotted lines in Figure 1) outline the band of uncertainty of the rate coefficient in the whole temperature range. The distance of the extreme values from the mean line is calculated in 100 K intervals. These distances provide “empirical” uncertainty parameters f .

(iv) The $f - T$ pairs of points are fitted using the following expression [16], [17]:

$$f(T) = \frac{3}{\ln 10} \sigma_{\kappa}(T)$$

$$\sigma_{\kappa}^2(T) = \sigma_{\alpha}^2 + \sigma_n^2 T^{-2} + \sigma_{\varepsilon}^2 \ln^2 T - 2r_{\alpha n} \sigma_{\alpha} \sigma_n T^{-1} - 2r_{\alpha \varepsilon} \sigma_{\alpha} \sigma_{\varepsilon} \ln T - 2r_{n \varepsilon} \sigma_n \sigma_{\varepsilon} T^{-1} \ln T + 2r_{\alpha n} \sigma_{\alpha} \sigma_n \ln T \quad (1)$$

The notations here refer to transformed parameters $\kappa(T) := \ln\{k(T)\}$, $\alpha := \ln\{A\}$ and $\varepsilon = E/R$, related to the following linearized form of the modified Arrhenius equation:

$$\kappa(T) = \alpha + n \ln\{T\} - \varepsilon T^{-1}$$

Since $f(T)$ is estimated at many temperatures, using equation (1) the six parameters of the covariance matrix (variances σ_{α} , σ_n , σ_{ε} and correlation coefficients $r_{\alpha n}$, $r_{\alpha \varepsilon}$, $r_{n \varepsilon}$) can be determined by parameter fitting, taking into account the following constraints:

$$0 \leq \sigma_{\alpha}, \sigma_n, \sigma_{\varepsilon}, \quad -1 \leq r_{\alpha n}, r_{\alpha \varepsilon}, r_{n \varepsilon} \leq +1,$$

$$0 \leq 1 - r_{\alpha n}^2 - r_{\alpha \varepsilon}^2 - r_{n \varepsilon}^2 + 2r_{\alpha n} r_{\alpha \varepsilon} r_{n \varepsilon}.$$

Step (iii) is very human time consuming and therefore a MATLAB code was written to carry out it in a semiautomatic way. All considered direct measurements and theoretical results are stored in a data file using a format, which is similar to the one used in the NIST database [13] on the summary page for a given reaction. Data for the reverse reaction were also collected and the corresponding Arrhenius parameters were transformed to the forward reaction ones using the thermodynamic data. These Arrhenius parameters were also stored in the data file. The data file also contains the Arrhenius parameters of the mean rate coefficient expression. The code then calculates the symmetrical k^{\min} and k^{\max} limits using any given ΔT resolution. The extremely outlying and therefore presumable wrong Arrhenius expressions can be eliminated in an interactive way and the program calculates the *a priori* covariance matrix of the Arrhenius parameters from the remaining data.

The determination of the domain of uncertainty is demonstrated on the example of reaction R2: H + O₂ + M = HO₂ + M. This reaction is one of the most important elementary reactions in the hydrogen combustion kinetics. For the low pressure limit, Baulch *et al.* [14] recommended Arrhenius parameters

$A = 6.89\text{E}+18 \text{ cm}^6 \text{ mol}^{-2} \text{ s}^{-1}$, $n = -1.20$ and $E/R = 0 \text{ K}$. We found about 60 articles dealing with experimental or theoretical determination of the rate coefficient of this elementary reaction. However, some of the collected rate expressions (mainly derived in the 1960's) were clearly outliers and were not considered. We finally used 9 experimentally determined and one theoretically derived rate coefficient expressions in the forward direction for Ar bath gas and 10 experimentally and two theoretically obtained expressions for N_2 bath gas. These expressions were used together to outline the uncertainty band of the rate coefficient by assuming 3rd body collision efficiency $m=0.5$ (Ar relative to N_2). As Figure 1 shows, these values outline well the band of uncertainty of the rate coefficient. In the temperature range between 300 K and 2000 K, at every 100 K the distance between the main value and the extreme values were calculated (see the dots in Figure 2) and the obtained f - T points were fitted using equation (1) yielding the elements of the *a priori* covariance matrix of Arrhenius parameters $\ln A$, n , and E/R . This matrix defines the range of uncertainty of the Arrhenius parameters and can also be used for the calculation of the $f(T)$ function using equation (1).

Konnov [2] suggested $f=0.08$ temperature-independent uncertainty parameter for this reaction, while Baulch *et al.* [14] assumed $f = 0.1$ at 298 K rising to 0.2 at 2000K. Our uncertainty limits are wider, and change between 0.19 (at 700 K) and 0.39 (at 2000 K).

The same procedure was carried out also with the other reactions (R1, R3–R8), and the *a priori* covariance matrix of each set of Arrhenius parameters was determined. Figure 3 shows for each reaction step the $f(T)$ values (symbols) as determined from the uncertainty bands of the rate coefficients and the $f(T)$ function (solid line), calculated from the *a priori* covariance matrix of the Arrhenius parameters.

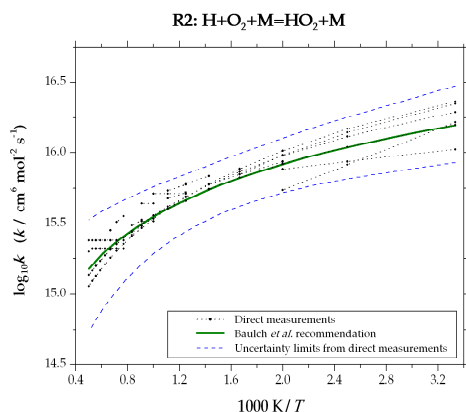


Fig. 1. Reaction R2: $\text{H} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$. The solid green mean line belongs to the recommended rate coefficient, the dashed blue lines are the upper and lower uncertainty limits, while the dots and the dotted lines belong to the individual direct measurements or theoretical calculations.

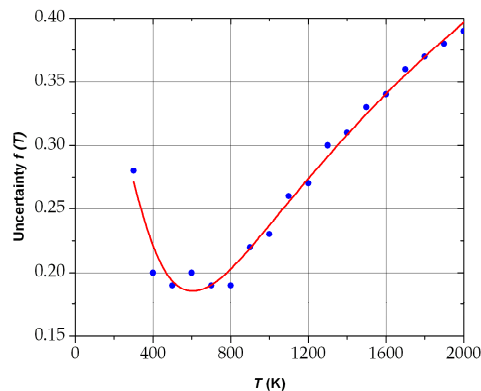


Fig. 2. Reaction R2: $\text{H} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$. The dots reflect the distance between the mean line and the extreme values, while the solid red line is the $f(T)$ uncertainty parameter calculated from the *a priori* covariance matrix of the Arrhenius parameters.

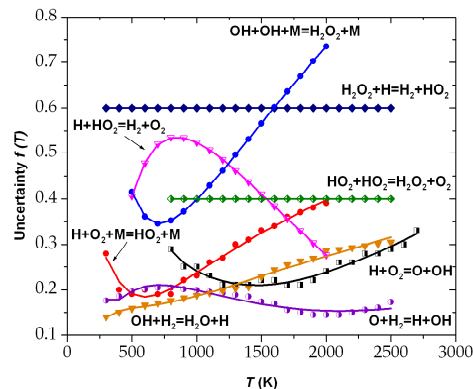


Fig. 3. For each optimised reaction step, the symbols show the $f(T)$ values at every 100 K, as determined from the uncertainty bands of the rate parameters and the solid line shows the $f(T)$ function, calculated from the *a priori* covariance matrix of the Arrhenius parameters.

In a similar way, the third body collision efficiency of Ar relative to N_2 in reaction R2 was collected from various literature sources, and its mean value and *a priori* range of uncertainty was determined.

Collection of relevant direct measurement data

The next step was the collection of direct measurement data for the selected reactions. The aim of direct measurements is the determination of the rate coefficient of a single reaction step at various temperatures, pressures and maybe using different bath gases. The reporting articles provide the values of the measured rate coefficients at the conditions of the experiment. Table 1 shows the number of direct measurements data points found for reaction steps R1 to

R8. All direct measurement results (*i.e.* rate coefficient values) were also encoded in PrIME file format [11]. This allowed for a uniform handling of all experimental data.

Table 1. Summary of the direct measurement data used at the optimisation

reaction	Number of data points	Number of datasets
R1	745	9
R2 (N ₂ bath gas)	40	4
R2 (Ar bath gas)	154	6
R3	338	10
R4	181	6
R5	72	4
R6 (Ar bath gas)	113	6
R7	–	–
R8	28	1

Parameter optimisation

Parameter optimisation was achieved by a minimization of an appropriate objective function. In this work the following objective function was used:

$$E_i = \frac{1}{N_i} \sum_{j=1}^{N_i} \left(\frac{Y_{ij}^{\text{mod}} - Y_{ij}^{\text{exp}}}{\sigma(Y_{ij}^{\text{exp}})} \right)^2$$

$$E = \frac{1}{N} \sum_{i=1}^N E_i \quad (2)$$

where

$$Y_{ij} = \begin{cases} y_{ij} & \text{if } \sigma(y_{ij}^{\text{exp}}) \approx \text{constant} \\ \ln y_{ij} & \text{if } \sigma(\ln y_{ij}^{\text{exp}}) \approx \text{constant} \end{cases}$$

Here N is the number of datasets and N_i is the number of data points in the i -th dataset. Values y_{ij}^{exp} and $\sigma(y_{ij}^{\text{exp}})$ are the j -th data point and its standard deviation, respectively, in the i -th dataset. The experimental data can be an ignition delay time or concentration (measured in an indirect experiment), or a rate coefficient (determined in a direct experiment). For the indirect measurement data, the simulated (modelled) value is Y_{ij}^{mod} , which is obtained from a simulation using an appropriate detailed mechanism. For the direct measurements, the corresponding modelled value Y_{ij}^{mod} is calculated using the appropriate expression for the determination of the rate coefficient at a given temperature, pressure and bath gas composition. $Y_{ij} = y_{ij}$, if the experiments have absolute error (independent of the value of y_{ij}); we used this option for the measured concentrations. We used option $Y_{ij} = \ln(y_{ij})$, if the experiments have relative error (proportional to the value of y_{ij}), which is characteristic for ignition time and rate coefficient measurements.

Fitting all parameters at the same time would mean fitting 23 parameters to about 2800 data points, which is a very challenging task computationally. Therefore, those simulated indirect data points were identified that are highly sensitive to the rate parameters of reactions R1 and R2 only. First, the rate parameters of these two reactions were fitted only to the corresponding data points. Then, the simulated data points sensitive to the rate parameters of reactions R1, R2 and R3 only were determined and the rate parameters of these three reactions were fitted to the related data points. This way, the number of fitted parameters and the considered data points were gradually increased, till all data points and all parameters were taken into account.

The *a posteriori* uncertainty of the parameters

The covariance matrix of all fitted parameters can be calculated from the variances of the experimental data points by taking into account the sensitivity of the simulated data points with respect to the optimised rate parameters. The detailed theory was described in our previous article [6]. This covariance matrix characterizes the *a posteriori* joint domain of uncertainty of the parameters. This uncertainty information is much better established than the previously determined *a priori* uncertainty, since now the information content not only of the direct, but also of the indirect measurements are taken into account. This covariance matrix can be transformed to the $f(T)$ *a posteriori* uncertainty function for each important reaction step, although due to the transformation important information about the correlation of the rate coefficients is lost. This temperature-dependent correlation also can be deduced from the covariance matrix [6].

Our optimisation code guarantees that the optimised rate coefficient – temperature functions remain within their *a priori* uncertainty limits. For each reaction step, the *a priori* and the *a posteriori* uncertainty limits were compared. In each case the *a posteriori* uncertainty range was much narrower and it was always well within the *a priori* uncertainty limits. This shows that the mechanism optimisation process resulted in a more precise and more detailed characterization of the uncertainty of the rate parameters. While the *a priori* uncertainty limits reflect the results of all consistent direct measurements and theoretical calculations, these do not take into account the information of the indirect measurements. The *a posteriori* uncertainty limits can be considered as the best estimation of the joint uncertainty of the optimised rate parameters, since these are based on all relevant direct and indirect measurement data.

As an example, Figure 4 compares the *a priori* and *a posteriori* ranges of uncertainty of the rate coefficients as a function of temperature on an Arrhenius plots for reaction R2: $\text{H} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$. The mean value of the rate coefficient (*i.e.* the centreline of the *a priori* uncertainty domain) is calculated from the expression recommended by Baulch et al. [14]. Derivation of the *a*

a priori uncertainty limits have been presented in Figures 1 and 2. The optimised rate expression and the narrow *a posteriori* uncertainty limits were results of the optimisation calculations.

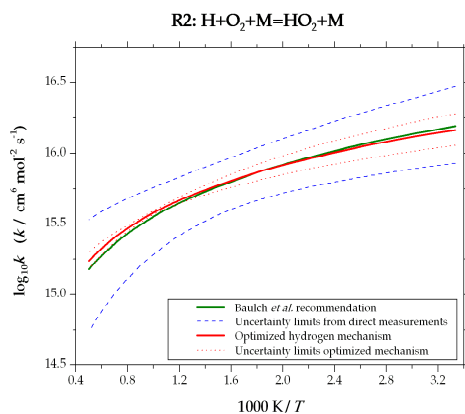


Fig. 4. The *a priori* and *a posteriori* ranges of uncertainty of the rate coefficients as a function of temperature for reaction R2: $\text{H} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$. Green solid line: the initial value of the rate coefficient before optimisation. Blue dashed lines: its *a priori* uncertainty limits. Red solid line: the optimised rate coefficient. Red dashed lines: the *a posteriori* uncertainty limits of the optimised rate coefficient.

Investigation of the optimised mechanism

The performance of the optimised mechanism was compared to 18 hydrogen combustion mechanisms that were mainly published in the last decade. The mechanisms used for comparisons included the recently published hydrogen combustion mechanisms of Ó Conaire *et al.* [1], Konnov [2], Hong *et al.* [3] and Burke *et al.* [4]. The other mechanisms [5, 7, 9, 18-25] were originally developed for wet CO, hydrocarbon or oxygenate combustion. The hydrogen combustion part of these mechanisms was used here.

Figure 5 shows the performance of all these mechanisms for the reproduction of all collected indirect measurement data (including the flame velocity measurements). The y-axis contains the value of objective function E as defined in equation (2). The figure shows that there is only a small improvement of the performance of the mechanisms over the years. For a more detailed comparison of these hydrogen combustion mechanisms please look at our recent paper [26]. The optimised mechanism derived here provides simulation results with the smallest deviation from the indirect experimental data, although its performance is not much better than those of several other recently published mechanisms.

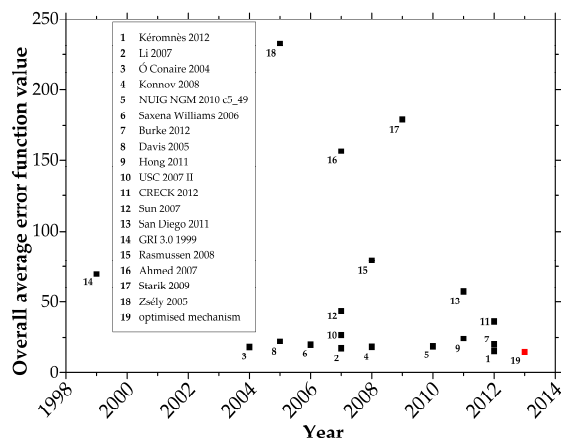


Fig. 5. Comparison of the performance of the optimised mechanism against 18 reaction mechanisms published since 1999. The optimised mechanism (number 19) provides simulation results that have the smallest deviations from the experimental data.

Conclusions

An optimisation of the hydrogen combustion mechanism of Kéromnès *et al.* [5] is presented here. A large amount of experimental data were collected from the literature on ignition delay time, jet-stirred reactor and flame velocity measurements. The aim was to collect all good quality indirect experiment data for hydrogen combustion. The local sensitivity coefficients of the simulated experimental data points were determined and the results indicated that the rate parameters of 8 reactions (in total 22 Arrhenius parameters and one 3rd body collision efficiency) have high influence on the simulation results. All direct measurements and theoretical determinations belonging to these 8 elementary reactions were collected and these values outlined the *a priori* uncertainty domain of the rate parameters. The optimisation took into account both the direct and indirect measurements and yielded the optimised values of these parameters, which are the best accordance with all available experimental data. The optimisation also provided the *a posteriori* uncertainty domain of the parameters, which is much smaller than the *a priori* one. The optimised mechanism, which differs from the Kéromnès *et al.* mechanism [5] in the values of the optimised rate parameters only, now provides the best reproduction of all collected indirect measurement values.

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