

Mechanism Reduction-Assisted Kinetic Parameter Optimization for the n-Pentanol Chemistry of the NUIGMech Multifuel Combustion Mechanism

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Abstract

Among renewable combustible fuels, n-pentanol is considered as a potential candidate. In this work, we proposed and applied a novel mechanism reduction-assisted procedure to optimize rate parameters of the recently developed n-pentanol part of the detailed NUIGMech 1.1 multifuel combustion kinetic mechanism, which would be otherwise unfeasible. According to our proposed method, first a precise reduced mechanism is developed, which thus can be optimized effectively against experimental targets, then the tuned parameter values are inserted back into the detailed model, whose accuracy thereby can also be improved to a similar extent.

Introduction

Our modern society relies on the large-scale consumption of energy: Our household appliances, working tools, services, and methods of transportation are working via the power of electricity or direct burning of fuel. Today, energy production is still overwhelmingly dominated by the combustion of fossil fuels, whose resources, according to some more pessimistic outlooks, may be depleted within half a century at the current rate of utilization.

Popularly considered renewable alternative to transportation fuels are bioalcohols. Bioethanol is already in use as a petrol additive in most countries (e.g. E10 fuel standard), and in certain countries (e.g. Brazil) as the main fuel component. However, the hygroscopic property of ethanol causes limited mixing with petroleum fuels, and may also cause corrosion in the fuel system. For this reason, longer chain bioalcohols are considered as a viable alternative, however their production is not economical yet. Larger bioalcohols like n-butanol and n-pentanol are expected to be better ingredients, as due to their longer carbon chains their physical and combustion properties are more similar to those of hydrocarbons fuel. Regarding the combustion of the long chain bioalcohols, biobutanol have already been researched for more than a decade, whereas on n-pentanol combustion still relatively little is known.

Kinetic models are developed for the understanding the combustion of fuels and to promote the development of new combustion technologies based on them. These kinetic models contain not only the reaction steps, but also their rate parametrization, which in theory defines their pressure and temperature dependence. Furthermore, thermodynamic and transport data is provided for each chemical species with the models, thus in theory it allows simulations of systems with complex geometries. Nowadays, computational fluid dynamics (CFD) simulations using chemical kinetic models are central tools in the development of modern combustion devices.

The models are then validated against data from indirect experimental measurements, whose results can be simulated using only detailed mechanisms, that is they contain indirect information on the rate of elementary reactions. Such experimental measurements are for example ignition delay times (IDT) measured in rapid compression machines (RCM) and shock tubes (ST), concentration data from jet-stirred reactor (JSR) measurements, and laminar burning velocities (LBV) from burners, etc.

The size of detailed combustion mechanisms, depending on the fuel molecule can range from tens of species and reactions (hydrogen, methane) to hundreds (natural gas, gasoline surrogates) and thousands (e.g. diesel surrogates, biodiesel). The accuracy of these models can be significantly improved by systematic parameter tuning, however, their sheer size makes their application unfeasible not only in CFD simulations, but also for parameter tuning against large amount of experimental data.

The aim of the present work is to improve the accuracy of the novel n-pentanol part of the NUIGMech multifuel mechanism (almost 3000 species and over 10000 reactions) against experimental wide range of experimental data. To overcome this very challenging task, we propose the novel concept of mechanism reduction-assisted parameter optimization.

In the following chapters, we introduce the combustion mechanism and experimental data collection used as targets in the mechanism optimization. Then we discuss the mechanism reduction procedure and the optimization procedure, and finally the validation of the optimized detailed mechanism.

The investigated combustion mechanism

The NUIGMech 1.1 combustion mechanism [1] is designed to incorporate description for the combustion of a wide array of fuels: from hydrogen, syngas and saturated and unsaturated C₁-C₅ hydrocarbons to

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formaldehyde, acetaldehyde, dimethyl-ether and C₁-C₄ alcohols. This mechanism has been recently extended with detailed chemistry for n-pentanol [2], which however, cannot be used separately due to the hierarchical structure of combustion pathways of fuel molecules of increasing size. Such multifuel mechanisms represent the state of art combustion knowledge as most of their rate coefficients have been consistently constrained by large number of experimental targets for various fuels as they were developed in a hierarchical manner over decades. Their further advantage is that they also allow the simulation of fuel blends, which are becoming more and more important in the future as the renewable fuels cover several compound types.

Combustion mechanism of such multifuel mechanisms, however, necessarily require several hundreds of species and reactions steps, thus their simulation can be a very time consuming even when a single fuel is investigated. The NUIGMech1.1 with the n-pentanol chemistry extension contains 2831 species and 11680 mechanisms, which can pose some serious difficulties in parameter optimization against an extensive data collection covering wide range of conditions.

Experimental data collection

Three types of experiment data are used as targets in the mechanism optimization: ignition delay times (IDT) from high-pressure shock tubes (HPST) and rapid compression machines (RCM) from the work of Chatterjee et al. [2], stationary concentration data from jet-stirred reactors (JSR) by Pelucchi et al. [3] and Togbé et al. [4], and laminar burning velocities (LBV) from spherical bomb measurements by Nativel et al. [5] Table 1 summarizes the covered ranges of conditions and the sizes of the data collections of various types. The JSR experiments provided stationary concentrations for several species O₂, CH₄, CH₂O, CO, CO₂, C₂H₂, C₂H₄, CH₃CHO, C₃H₆, C₄H₆, C₄H₈₋₁, n-C₅H₁₁OH, C₅H₁₀₋₁, P-C₄H₉CHO by Togbé

et al., whereas Pelucchi et al. measured concentrations also for H₂, H₂O and C₂H₆.

All experimental conditions and measured data we collected were stored in ReSpecTh Kinetics Data (RKD) XML data files [6], which allow their automated use for setting up simulations in the Optima++ parameter optimization environment [7]. Our data collection is very unbalanced one as it contains 104 series of concentration, 14 series of ignition delay, and only 3 series of laminar burning velocity measurements. Within a data series a single condition parameter is changed systematically: temperature for JSR and IDT measurements, and equivalence ratio for LBV measurements, thus we introduced a weighting in the error function to get an optimized mechanism with balanced performance for the three data types.

The total error of each experimental data series was estimated based on the error value given by the experimentalists and the inherent statistical noise of the data series using the following formula:

$$\sigma_{\text{exp,tot}}^2 = \sqrt{\sigma_{\text{exp}}^2 + \sigma_{\text{stat}}^2} \quad (1)$$

The reported experimental error was taken as $2\sigma_{\text{exp}}$ unless it was stated differently in the original publication. For JSR simulation, the reported uncertainty was given in 5-10% was given, which, however cannot be interpreted for zero measured values and would lead to strong overweighting of tiny concentration values in the error function. Thus, we took as a rule thumb we took σ_{exp} as the 10% of the maximum value of the measured concentration of the corresponding species within each data series. The used values of uncertainties during the optimization are listed in Table 1. Beyond these estimates, we also assessed the scatter of the statistical noise (σ_{stat}) for each data series was determined with the help of the Minimal Spline Fit code [8]. The minimal spline fit code generates an optimal trendline in the form of

Table 1. The indirect experimental data collection used as target in the mechanism optimization

data type	ignition delay times (IDT)		stationary concentrations		laminar burning velocities (LBV)
method	high-pressure shock tube (HPST)	rapid compression machine (RCM)	jet-stirred reactor (JSR)		spherical bomb
authors	Chatterjee et al.		Pelucchi et al.	Togbé et al.	Nativel et al.
equivalence ratio	0.5, 1, 2	0.5, 1, 2	0.5, 1, 2	0.35, 0.5, 1, 2	0.7 - 1.3
pressure (atm)	15, 30	15, 30	1	10	1
temperature (K)	800-1250	670-950	500-1100	770-1220	353, 433, 473
no. data files	6	8	3	4	3
no. data series	6	8	42	62	3
no. data points	49	36	1050	852	44
weights w_{f_S}	1/(6+8)		1/(42+62)		1/3
uncertainty σ_{exp}	10%		10% of its maximum concentration in the data series		1.2%

Akima splines that minimizes the Akaike information loss. The root mean square deviation of the data from this spline curve gives the σ_{stat} standard deviation of the statistical noise.

The novel concept of mechanism reduction-assisted parameter optimization

To speed up the parameter optimization of large reaction mechanism, which would otherwise be computationally too expensive or even unfeasible with current computational methods and resources, we propose the following mechanism reduction-assisted parameter optimization procedure:

1. Development of a reduced mechanism, which can accurately reproduce the simulation results of the large mechanisms at the conditions of the experimental targets.
2. Optimization of the important parameters of the reduced mechanism against the experimental targets.
3. Reintroduction of the optimal parameter values to the large mechanism and validation of this updated mechanism against the experimental targets.

Mechanism reduction procedure

Unfortunately, the full mechanism could not be simulated successfully at the experimental conditions of the targets using OpenSMOKE [9], thus we used Cantera [10] for the reference simulations and for the mechanism with the full mechanism. Therefore, in this work we applied, reaction rate-based mechanism reduction method by modification example code within Cantera. The mechanism reduction procedure is summarized in Fig. 1 and has the following steps:

1. Simulations are carried out at conditions covering those of target experimental data and reaction rates (net rate for reversible reactions) were calculated and stored at each solution state, namely at each grid point, at frequent time points and at each stationary solution for LBV, IDT and JSR simulations, respectively.
2. The reactions rates at each stored state are normalized with respect to the largest absolute rate and the reactions are ranked according to this normalized value at each state. For reaction i the normalized reaction rate value at state j is:

$$R_{ij}^{\text{norm}} = \frac{|R_i(\text{state}_j)|}{\max_k |R_k(\text{state}_j)|} \quad (2)$$

3. Three global rankings are determined for the three simulation types based on the maximum values of

normalized rates of reactions over the states in the simulations of those experiments:

$$R_{i,\text{LBV}}^{\text{norm}} = \max_{j:\text{LBV}} R_{ij} \quad (3)$$

$$R_{i,\text{IDT}}^{\text{norm}} = \max_{j:\text{IDT}} R_{ij} \quad (4)$$

$$R_{i,\text{JSR}}^{\text{norm}} = \max_{j:\text{JSR}} R_{ij} \quad (5)$$

4. For LBV simulations, reactions are selected into the reduced mechanism in descending order of their $R_{i,\text{LBV}}^{\text{norm}}$ values until the mechanism reproduces the simulation results of the full mechanism within 5% accuracy.
5. For IDT simulations, reactions are selected into the reduced mechanism in descending order of their $R_{i,\text{IDT}}^{\text{norm}}$ values until the mechanism reproduces the simulation results of the full mechanism within 5% accuracy.
6. For JSR simulations, reactions are selected into the reduced mechanism in descending order of their $R_{i,\text{JSR}}^{\text{norm}}$ values until the mechanism reproduces the simulation results of the full mechanism within 5% accuracy.
7. If no inclusion was done to the mechanism in steps 5 or 6 then the steps from step 4 are repeated.

If no inclusion was done then we arrived at a reduced mechanism which can accurately reproduce the simulation results of the full mechanisms at the conditions of the target experimental data, thus they are expected to behave similarly upon parameter tuning, which allows indirect optimization of full mechanism.

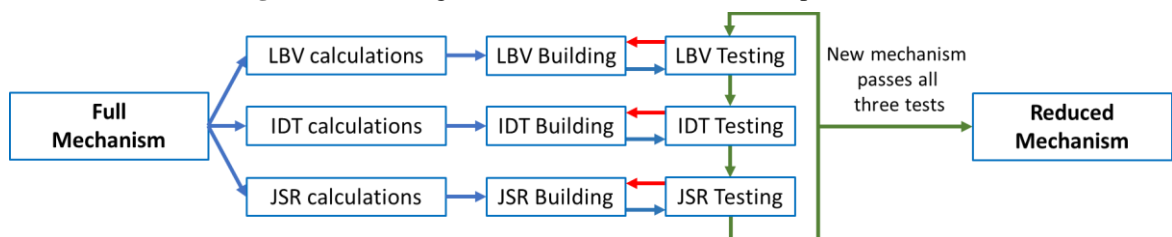
Mechanism optimization procedure

For the parameter optimizations, we applied code Optima++ [11], which implements the optimization method developed by Turányi et al. [12] and uses the numerical optimization algorithm FOCTOPUS developed by T. Nagy [12,13]. In this work we used OpenSMOKE++ [9,14] simulation code for IDT and JSR simulations and Zero-RK [15] for LBV simulations. The method minimizes the following error function:

$$E(\mathbf{P}) = \frac{1}{N} \sum_{f=1}^{N_f} \sum_{s=1}^{N_{fs}} \frac{w_{f,s,d}}{N_{f,s,d}} \sum_{d=1}^{N_{f,s,d}} \left(\frac{Y_{f,s,d}^{\text{sim}}(\mathbf{P}) - Y_{f,s,d}^{\text{exp}}}{\sigma_{f,s,d}^{\text{exp,tot}}} \right)^2, \quad (6)$$

where N is the total number of data series, N_f is the number of data files, N_{fs} is the number of data series in the f -th file and $N_{f,s,d}$ is the number of data in its s -th data series. In this data series, $Y_{f,s,d}^{\text{exp}}$ is the optionally transformed d -th data and $Y_{f,s,d}^{\text{sim}}$ is its simulated value,

Figure 1. Flow diagram of the mechanism reduction procedure



which depends on parameter vector \mathbf{P} that contains transformed Arrhenius parameters ($\ln A$, n , E/R). R is the universal gas constant. The w_{fsd} factors are the weights, which can help to develop optimized mechanism with balanced performance in reproducing all type of experimental data.

The experimental uncertainty of a data point is also taken into account via the $\sigma_{fsd}^{\text{exp,tot}}$ standard deviation of its determination (see Table 1). Thus, square root of $E(\mathbf{P})$ measures the root mean squared deviation of the simulation results from the experimental data relative to the standard deviation of the experimental data. Square root of $E(\mathbf{P})$ is around 1 for a perfect model, and below 3 for a model which is accurate on average within three experimental standard deviation.

The selected Arrhenius parameters were optimized in such a way that the rate coefficients calculated with the optimized rate parameters always remained within their prior uncertainty interval [$k_{\min}(T)$; $k_{\max}(T)$] in the temperature interval of 600 K to 3000 K. The uncertainty parameter is defined as the radius of a symmetric uncertainty range around the nominal $k^0(T)$ value on \log_{10} scale:

$$f_{\text{prior}}(T) = \log_{10} \frac{k_{\max}(T)}{k^0(T)} = \log_{10} \frac{k^0(T)}{k_{\min}(T)}. \quad (7)$$

As no a priori information was known for the uncertainty range of the influential reactions, one order of magnitude of uncertainty was assumed for the rate coefficients in the 600-3000K temperature range, which corresponded to $f_{\text{prior}} = 1$ value.

Selection of active parameters

Detailed combustion mechanisms usually contain large number of uncertain parameters. Frenklach et al. suggested that only those parameters ('the active parameters') that have a high influence on the simulated value of the experimental data need to be fitted. Frenklach et al. noted [16] that at the selection of the active parameters not the local sensitivity information, but the product of sensitivity and the range of parameter uncertainty should be considered.

In a recent work [17], Kovács et al. proposed a very efficient novel method, called PCALIN, which was derived from the incomplete second-order expansion of the error function in Eq. (1) by T. Nagy. The dominant contributions in the second-order term can be identified by principal component analysis (PCA) of a scaled local sensitivity matrix, which incorporates not only the local sensitivity coefficients with respect to pre-exponential factors:

$$\tilde{s}_{ij} = \frac{\partial Y_{fsd}^{\text{sim}}(\mathbf{P})}{\partial \ln A_j}, \quad (8)$$

but also considers the uncertainty of parameters (f), and the uncertainty ($\sigma_{fsd}^{\text{exp,tot}}$) and the weights (w_{fsd}/N_{fsd}) of the experimental data in the error function. The PCA identifies the most important correlated parameter groups (i.e. reaction groups) which should

be optimized together to efficiently reduced the values of the error function. The first-order variations of the error functions ("LIN" stands for linear contribution) due to parameter variations along a principal component can also be significant, which is also taken into account by the PCALIN selection procedure and can provide a very efficient selection of parameters. The PCALIN method is implemented in the Strategy code, which is also available from the ReSpecTh webpage [18].

Results

The size, the simulation speed and the accuracy of the original and optimized full and reduced mechanisms can be found Table 2 and also shown in Fig. 2. The reduced mechanism had only 322 species and 2831 reactions, while it could be simulated more than 40 times faster at homogeneous conditions (i.e. IDT and JSR), and had no or only minor convergence issues in laminar flame simulations opposed to the full mechanism. The reduced mechanism has the same accuracy as the full mechanism for all experimental data types: they both showed very little error for LBV simulations, and significant, on average 3.4 and 2.5 times larger error (i.e. \sqrt{E} values) than the experimental uncertainty for IDT and JSR targets, respectively.

We carried out brute-force local sensitivity analysis using the Optima simulation environment, which employed the OpenSMOKE [9,14] code for ignition and jet-stirred reactor simulations and the Zero-RK [15] code for laminar flame simulations.

Using local sensitivities, the experimental uncertainties and weights discussed in the Experimental data collection chapter (see Table 1 and text) and assuming $f_{\text{prior}} = 1$ value, the PCALIN method could identify 64 influential rate coefficients out of the 524 pentanol-related rate coefficients in the reduced mechanism. This rate coefficient included PLOG rate coefficients defined for various pressures.

The Optima++ code was used to optimize the $3 \times 64 = 192$ Arrhenius parameters of the identified rate coefficients while constraining their $k(T; A, n, E)$ Arrhenius curves within ± 1 order of magnitude wide band in the 600K-3000K temperature range around the initial Arrhenius curves. The same simulation codes were used here, as for sensitivity analysis.

Table 2. Size and performance of the mechanisms

	full		reduced	
	orig.	optimized	orig.	optimized
no. species	2831		322	
no. reactions all/pentanol	11680/631		2096/524	
0D simul. rate	1		~ 40	
\sqrt{E} for LBV	0.71	0.77	0.70	0.79
\sqrt{E} for IDT	3.38	1.92	3.37	1.92
\sqrt{E} for JSR	2.48	2.04	2.49	2.03
\sqrt{E} overall	2.45	1.68	2.45	1.68

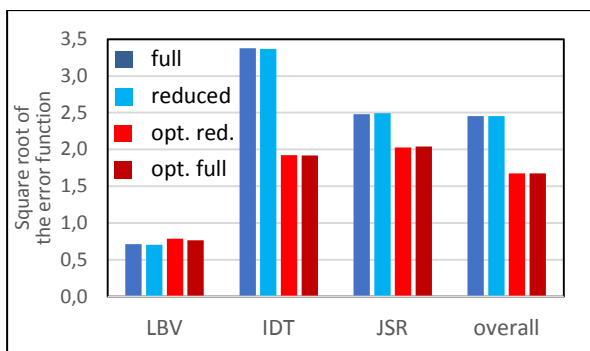


Figure 2. Accuracy of the mechanisms for various experimental data types

By the optimization the error function of the reduced mechanism for IDT and JSR targets could be reduced significantly on average, down to two standard deviations of experimental uncertainty, whereas the great accuracy for LBV targets did not deteriorate. By inclusion of the optimized parameters into the full mechanism, its accuracy could be improved exactly with the same extent. The accuracy of the mechanisms for LBV data, IDT data from RCMs and HPSTs, and concentration data from JSR's are shown in Figs. 3-6, respectively. In all cases, the accuracy of the reduced mechanism and optimized mechanism behave in accord with the expectations proving the transferability of optimized parameters.

In the case of JSR targets, lower improvements can be realized as in the case of IDT targets, which can be explained by the JSR data series containing concentrations for several small species, whose chemistry is largely affected by reactions that are not exclusive to *n*-pentanol, thus were not considered during the optimization. For LBV targets, since the error function was already very small, the reason for their inclusion into the optimization was to avoid the deterioration of the good performance for LBV data.

Conclusions, outlooks

The aim of this research was to improve the accuracy of the detailed *n*-pentanol chemistry of the NUIGMech 1.1 multifuel combustion mechanism. This task, due to the large size of the mechanism, is unfeasible by current computational methods and resources, thus we came up with the novel idea of mechanism reduction assisted parameter optimization. By mechanism reduction a much smaller, but accurate reduced mechanism could be made, which then could be optimized against wide range of experimental targets in a reasonable time. The marked improvement in the accuracy of the reduced mechanism could be realized in the huge NUIGMech mechanism as well by transferring the tuned parameter values to it, making this seemingly impossible task feasible. This powerful approach is expected to have great importance in the optimization of detailed large combustion mechanisms, whose number is rapidly growing due the advancement of automatic mechanism generation tools and increasing interest in renewable fuels.

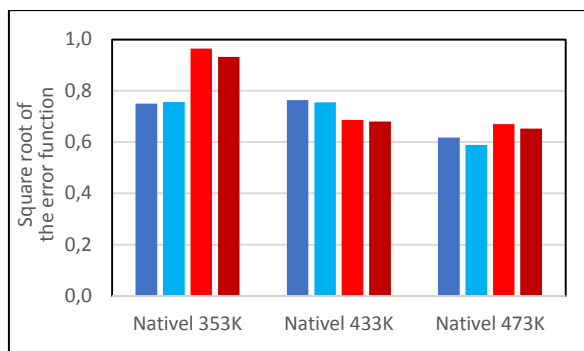


Figure 3. Accuracy of the mechanisms for laminar burning velocity (LBV) measurements (legend as in Fig. 2.)

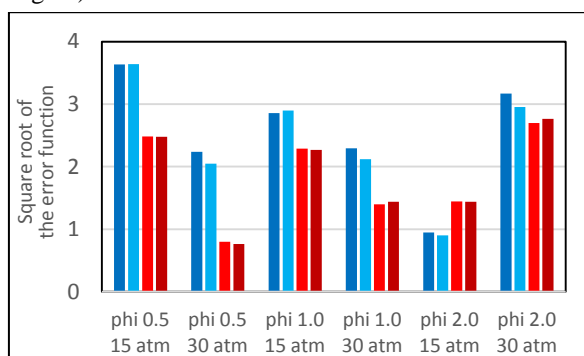


Figure 4. Accuracy of the mechanisms for ignition delay measurements in high-pressure shock tubes (HPST, Chatterjee et al., legend as in Fig. 2.)

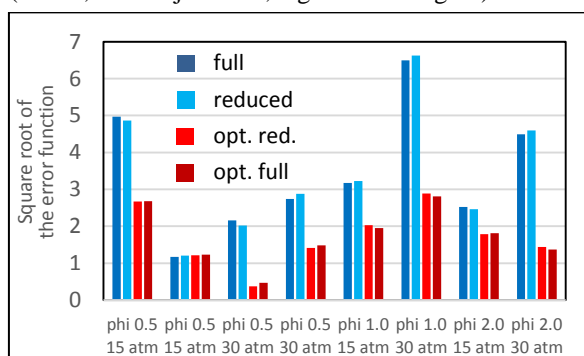


Figure 5. Accuracy of the mechanisms for ignition delay measurements in rapid compression machines (RCM) (Chatterjee et al.).

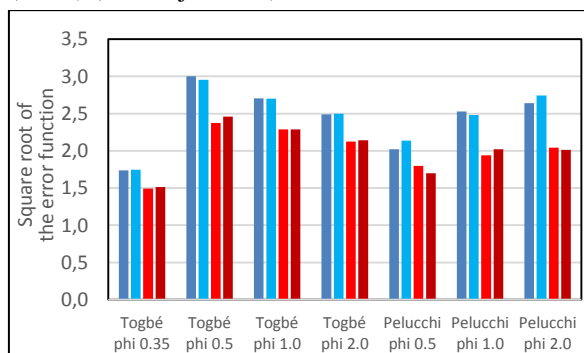


Figure 6. Accuracy of the mechanisms for concentration measurements in jet-stirred reactors (JSR, legend as in Fig. 5).

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