

Original Research

An optimized kinetic model for H₂-O₂ combustion in jet-stirred reactor at atmospheric pressure**Authors:**

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ABSTRACT:

An optimized kinetic model for hydrogen combustion in a jet-stirred reactor was proposed based on a validated mechanism. The rate constants were optimized using a genetic algorithm to minimize the prediction error of the outlet species' concentrations. The reference experimental data of jet-stirred reactor were selected from the literature. Optimization was established with and without constraints. Then, the kinetic models were evaluated using the relative errors in predicting the concentrations of major species at the outlet (H₂, O₂ and H₂O) and their accuracy in the calculation of ignition delay times. The comparison of experimental and calculated ignition delay time using unconstrainedly optimized model, rejected the optimization of kinetic model without any constraints. The optimized kinetic model showed a relatively better performance than the original model, especially under atmospheric conditions. At higher pressures and very rich conditions, the deviations from experimental data became greater than the original model.

Keywords:

Hydrogen combustion, genetic algorithm, jet-stirred reactor.

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INTRODUCTION

Hydrogen will play an important role as a future energy source. The kinetics of hydrogen combustion is very important in the design of combustion chambers with respect to equipment design, material selection, sizing and heat of reaction. Historically, H₂ is the first fuel whose combustion kinetic with oxygen has been studied (Westbrook *et al.*, 1984). In addition, the elementary reactions of H₂-O₂ systems play an effective role in the species pool, in combustion of any other hydrocarbon fuel (Mueller *et al.*, 1999). Despite the simplicity of the H₂ molecule, its list of combustion reactions has not been completed so far. Thus, there are still some remaining uncertainties in the kinetics of H₂ combustion (Konnov, 2008).

There are several kinetic models for the combustion and oxidation of H₂ in the literature. Olm *et al.* (2014) reviewed and tested one of the recent kinetic models of H₂ combustion against a comprehensive database of published experimental works. The mechanism of Konnov (2008) was within the most successful mechanisms. In contrast, Mével *et al.* (2012) examined the mechanisms of Konnov (2008), GRI-Mech 3.0 (1999) and Dagaut (Cong *et al.*, 2009) in simulation of Jet-Stirred Reactor (JSR) and reported that both Konnov's (2008) and GRI-Mech 3.0 (1999) mechanisms,

have weaknesses in prediction of the extinction condition in JSR. Hence, Dagaut's mechanism (2009) is the most reliable one.

Many combustion processes take place in atmospheric chambers, like process furnaces, boilers, space heaters, etc., using conventional fossil fuels that may also use H₂. Among the different apparatus for kinetic modeling (eg. shock tubes, internal combustion engines, premixed flamed, plug-flow reactor), it seemed that the JSR model due to its simplicity and flow regime, could well describe equipment like furnaces. Table 1 shows recent kinetic models of H₂ combustion and their applied apparatus as reference data for rate optimization.

There are large sets of experimental data for H₂ combustion using various apparatus (Olm *et al.*, 2014), but, unfortunately, JSR was seldom used for experimental works. A JSR is simple to establish practically and also has a simple mathematical model. Cong and Dagaut, (2009) published their data and model for oxidation of N₂-diluted H₂, H₂/CO₂, and H₂/CH₄ within a JSR.

The main objective of this study was to optimize the rate parameters of a selected mechanism against only the experimental JSR data and evaluate the original and optimized versions. The assessment and comparison criteria consist of relative errors of major species

Table 1. Recent mechanisms for H₂ combustion and their apparatuses for rate optimization

No.	Mechanism	Target Fuel	Reference data for rate optimization			Reference
			Ignition	Flow Reactor	Flame Speed	
1	Kéromnès-2013	H ₂ and Syngas	ü	-	-	Kéromnès <i>et al.</i> (2013)
2	Metcalfé-2013	H ₂ /CO/C ₁ -C ₂	ü	-	ü	Metcalfé <i>et al.</i> (2013)
3	Hong-2011	H ₂	ü	ü	-	Hong <i>et al.</i> (2011)
4	NUIG-NGM-2010	Natural Gas	ü	-	-	Healy <i>et al.</i> (2010)
5	USC-II	H ₂ /CO/C ₁ -C ₄	ü	ü	ü	Wang <i>et al.</i> (2007)
6	Starik-2009	Syngas	ü	-	ü	Starik <i>et al.</i> (2010)
7	Dagaut-2009	H ₂ /CO/CH ₄	-	ü	-	Le Cong <i>et al.</i> (2009)
8	Rasmussen-2008	H ₂ /CO	-	ü	-	Rasmussen <i>et al.</i> (2008)
9	Sun-2007	H ₂ /CO	-	-	ü	Sun <i>et al.</i> (2007)
10	Saxena-2006	H ₂ /CO	-	-	ü	Saxena <i>et al.</i> (2006)
11	Davis-2005	H ₂ /CO	ü	ü	-	Davis <i>et al.</i> (2005)
12	Zsély-2005	H ₂ /CO	ü	-	-	Zsély <i>et al.</i> (2005)
13	Conaire-2004	H ₂	-	ü	-	Conaire <i>et al.</i> (2004)
14	Li-2004	H ₂	-	ü	-	Li <i>et al.</i> (2004)

Table 2. Elementary reactions in Konnov's mechanism (2008) and their original and optimized rate parameters for H₂/O₂ combustion system

No.	Reaction	Original Rate Constants			Optimized Rate Constants		
		k ₀ [*]	β	E _a ^{**}	k ₀ [*]	β	E _a ^{**}
R1	H + H + M = H ₂ + M ^a	7.00E+17	-1	0	2.20E+19	-1.76	0
R2	H + H + H ₂ = H ₂ + H ₂	1.00E+17	-0.6	0	3.10E+18	-1.20	0
R3	H + H + N ₂ = H ₂ + N ₂	5.40E+18	-1.3	0	2.09E+19	-0.97	0
R4	H + H + H = H ₂ + H	3.20E+15	0	0	2.74E+17	0	0
R5	O + O + M = O ₂ + M ^a	1.00E+17	-1	0	8.70E+18	-1.91	0
R6	O + H + M = OH + M	6.75E+18	-1	0	4.83E+20	-0.55	0
R7	H ₂ O + M = H + OH + M ^a	6.06E+27	-3.312	120770	9.64E+27	-5.29	143951
R8	H ₂ O + H ₂ O = H + OH + H ₂ O	1.00E+26	-2.44	120160	7.25E+27	-1.82	133628
R9	H + O ₂ + M = HO ₂ + M ^{a,b}	4.66E+12	0.44	0	8.92E+13	0.56	0
R10	H + O ₂ + Ar = HO ₂ + Ar ^b	4.66E+12	0.44	0	8.70E+13	0.76	0
R11	H + O ₂ + O ₂ = HO ₂ + O ₂ ^b	4.66E+12	0.44	0	5.38E+12	0.68	0
R12	H + O ₂ + H ₂ O = HO ₂ + H ₂ O ^b	9.06E+12	0.2	0	5.94E+14	0.25	0
R13	OH + OH + M = H ₂ O ₂ + M ^{a,b}	1.00E+14	-0.37	0	4.97E+15	-0.21	0
R14	OH + OH + H ₂ O = H ₂ O ₂ + H ₂ O ^b	1.00E+14	-0.37	0	5.63E+15	-0.29	0
R15	O + H ₂ = OH + H	5.06E+04	2.67	6290	3.45E+06	1.60	9029
R16	H + O ₂ = OH + O	2.06E+14	-0.097	15022	1.07E+16	-0.15	22638
R17	H ₂ + OH = H ₂ O + H	2.14E+08	1.52	3450	2.13E+10	1.09	4093
R18	OH + OH = H ₂ O + O	3.34E+04	2.42	-1930	2.15E+06	4.50	-2549
R19	HO ₂ + O = OH + O ₂	1.63E+13	0	-445	1.47E+15	0	-742
R20	H + HO ₂ = OH + OH	1.90E+14	0	875	6.64E+15	0	1685
R21	H + HO ₂ = H ₂ O + O	1.45E+12	0	0	9.42E+13	0	0
R22	H + HO ₂ = H ₂ + O ₂	1.05E+14	0	2047	3.31E+15	0	3700
R23	H ₂ + O ₂ = OH + OH	2.04E+12	0.44	69155	1.32E+14	0.85	104315
R24	HO ₂ + OH = H ₂ O + O ₂ ^c	2.89E+13	0	-500	1.68E+15	0	-454
R25	HO ₂ + OH = H ₂ O + O ₂ ^c	9.27E+15	0	17500	6.51E+17	0	10615
R26	HO ₂ + HO ₂ = H ₂ O ₂ + O ₂ ^c	1.03E+14	0	11040	5.35E+14	0	13313
R27	HO ₂ + HO ₂ = H ₂ O ₂ + O ₂ ^c	1.94E+11	0	-1409	5.34E+10	0	-1629
R28	HO ₂ + HO ₂ + M = H ₂ O ₂ + O ₂ + M	6.84E+14	0	-1950	2.14E+16	0	-1042
R29	H ₂ O ₂ + H = HO ₂ + H ₂	1.70E+12	0	3755	1.69E+14	0	1897
R30	H ₂ O ₂ + H = H ₂ O + OH	1.00E+13	0	3575	9.45E+13	0	6916
R31	H ₂ O ₂ + O = HO ₂ + OH	9.55E+06	2	3970	8.97E+08	1.23	6086
R32	H ₂ O ₂ + OH = HO ₂ + H ₂ O ^c	2.00E+12	0	427	2.52E+13	0	459
R33	H ₂ O ₂ + OH = HO ₂ + H ₂ O ^c	1.70E+18	0	29400	1.66E+20	0	41828

* in mole-cm-sec-K;

** in cal/mole;

^a Includes third-body efficiency;^b The fall-off behavior of this reaction is expressed in the form as expressed by Troe's equation (Gilbert *et al.*, 1983);^c Duplicated reaction for two temperature ranges.

concentrations (H₂, O₂ and H₂O) at a JSR outlet, comparison of the rate constants of major reactions and prediction of ignition delay times in a shock tube.

MATERIALS AND METHODS

Combustion Mechanisms

The skeletal reactions and the thermophysical properties data for species (eg. enthalpy of formation and heat capacity) of Konnov's mechanism (2008) were

used. The rate parameters of this mechanism were optimized to fit the JSR experimental data of H₂ oxidation. Thus, a new optimized mechanism with the same skeletal reactions was generated. Table 2 illustrates the elementary reactions and rate parameters of both mechanisms.

The mathematical model of the Perfectly-Stirred Reactor (PSR) in CANTERA (Goodwin, 2011) was used in two stages of this study: (1) in the simulation of

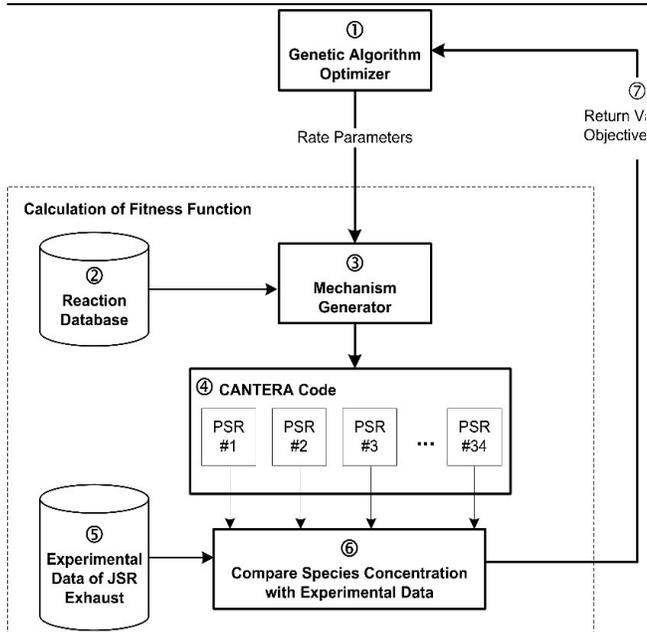


Figure 1. Optimization flowchart used for each mechanism.

perfectly-stirred reactor during mechanism optimization, and (2) in the prediction of ignition delay time in the evaluation of the optimized mechanism. The Perfectly-Stirred Reactor (PSR) required steady-state conditions for a flow reactor. In contrast, in the prediction of ignition delay time, the CANTERA code was used in a time-dependent (transient) mode for a closed batch reactor.

Optimization Methodology

Decision Variables

A kinetic model comprises of a set of elementary reactions, with corresponding rate parameters of the modified Arrhenius equation (k_0 , β , E_a) as expressed in Eq. 1.

$$k = k_0 T^\beta \exp\left(\frac{-E_a}{RT}\right) \quad (1)$$

Several methods have been proposed in the literature to estimate kinetic parameters, including the studies done by Willems *et al.* (1988) and Frenklach *et al.* (1992). Recently, by increasing the popularity of evolutionary algorithms such as Genetic Algorithm

(GA), the potentials of GA in estimating kinetic parameters became attractive. Detailed reviews could be found in the literature (Elliott *et al.*, 2004; Wei *et al.*, 2011).

The structure of optimization code and its flowchart used in this work is shown in Figure 1. The evolutionary algorithm, NSGA-II (Non-dominated Sorting Genetic Algorithm II) by Deb *et al.* (2002), was used for this study (Step 1 in Figure 1). The objective/fitness function of the optimization is the sum of relative errors as described in Section 2.3.2 in details. A mechanism file (input file) with randomly selected rate parameters was generated, using skeletal reactions in database and the generated kinetic parameters by GA (Step 3 in Figure 1). By using the mechanism file, all 34 predefined operating conditions of JSR of Cong and Dagaut, (2009) were simulated in step 4 of Figure 1. The experimental data of the outlet concentrations were saved in another database (Part 5 of Figure 1), so by calculation of species concentrations in the JSR outlet using that mechanism, the objective function could be calculated (Step 6 of Figure 1).

Objective Function

Objective/fitness function in this study was defined as the accuracy of combustion model (both kinetic and reactor models) in prediction of outlet concentration of JSR. It was calculated by summing relative errors between the calculated mole fractions and their corresponding experimental mole fractions, which is expressed in Eq. 2:

$$\text{Objective Function} = \left(\sum_{i=1}^n \frac{|y_{i,calc} - y_{i,meas}|}{y_{i,meas}} \right) \times 100 \quad (2)$$

In equation 2, 'n' is the number of experiments, $y_{i,calc}$ is the calculated gas-phase mole fraction of species i using kinetic in each trial, $y_{i,meas}$ is the measured gas-phase mole fraction of species $y_{i,meas}$. The required value of $y_{i,calc}$ is obtained from simulation results. The mathematical model of the Perfectly-Stirred Reactor

Table 3. Methods and parameters used in GA.

Specifications/Methods	Value
Population	16
Cross-over method	Single-point
Cross-over probability	0.55
Mutation operator	bitwise
Mutation probability	0.01
Number of generations	1000
Number of bits for k_0	28
Number of bits for β	12
Number of bits for E_a	12

(PSR) in CANTERA (Goodwin, 2011) was used, in order to simulate the outlet conditions of the experimental JSR. The objective function of the generated mechanism with respect to experimental results were sent to the GA code as an objective function (Step 7 of Figure 1).

The population and breeding parameters of GA, selected based on the values proposed by Hedayatzadeh *et al.* (2014), are shown in Table 3. Also, the lower and upper bounds of each variable type is shown in Table 4.

Optimization Constraints

Optimizations were carried out in two scenarios: unconstrained and constrained. Unconstrained optimization implies an optimization without any constraint for limiting the objective function or simulation results. In this case, the valid domain for decision variables comprised the feasible region. In the constrained scenario, the feasible space was constrained by defining the lower and upper limits for the concentration of intermediate species. These species include: H, O, OH, HO₂ (hydroperoxyl) and H₂O₂ (hydroperoxide). These intermediate and unstable species were not measured by Cong and Dagaut, (2009) during the experiments. Therefore, the lower and upper limits were derived from simulations of each reactor condition using the mechanisms of Konnov (2008);

Table 4. Domain of each type of decision variables

Variable	Range
k_0	0.01 – 100 × (model's initial value)
B	0.5 – 2 × (model's initial value)
E_a	0.5 – 2 × (model's initial value)

Conaire *et al.* (2004), Dagaut (2009) and GRI-Mech 3.0 (1999). The constraints were applied to only five randomly selected cases from all 34 cases of reactor conditions.

RESULTS AND DISCUSSION

Due to the stochastic nature of GA, there is always an uncertainty in reaching the global optimum point. On the other hand, GA is a very time-consuming optimization method. Thus, each optimization was replicated 2 times and resulted in the same trend and final values. Figure 2 shows the trends of both unconstrained and constrained optimizations. The constrained optimization showed relatively slower convergence mainly due to the fewer number of feasible population in each generation.

The optimized and original rate parameters are illustrated in Table 2. Despite the same final objective values for both optimizations, the optimized variables are completely different. Figure 3 compare the rate constants for selected elementary reactions for Konnov's unconstrained and constrained optimized mechanisms.

Considering important reactions, the rate of R16 ($H + O_2 = OH + O$) remained unchanged, while the rate of R17 ($H_2 + OH = H_2O + H$) increased significantly. By decreasing the rate constant of R15 ($O + H_2 = OH + H$), it is obvious that the role of H in the chain branching reaction became higher than the O and OH radicals in the JSR conditions. Simultaneously, the rate constants of R7 ($H_2O + M = H + OH + M$) and R23 ($H_2 + O_2 = OH + OH$) as OH generator reactions fell extremely.

At the other side of the spectrum, most increments of the rate constants were related to R18 ($OH + OH = H_2O + O$), R6 ($O + H + M = OH + M$), and R25 ($HO_2 + OH = H_2O + O_2$). All of these reactions are chain terminators. This may indicate that the pool concentrations of radicals decreased due to the mixed regime of reacting flow within the reactor, which resulted in more chain termination.

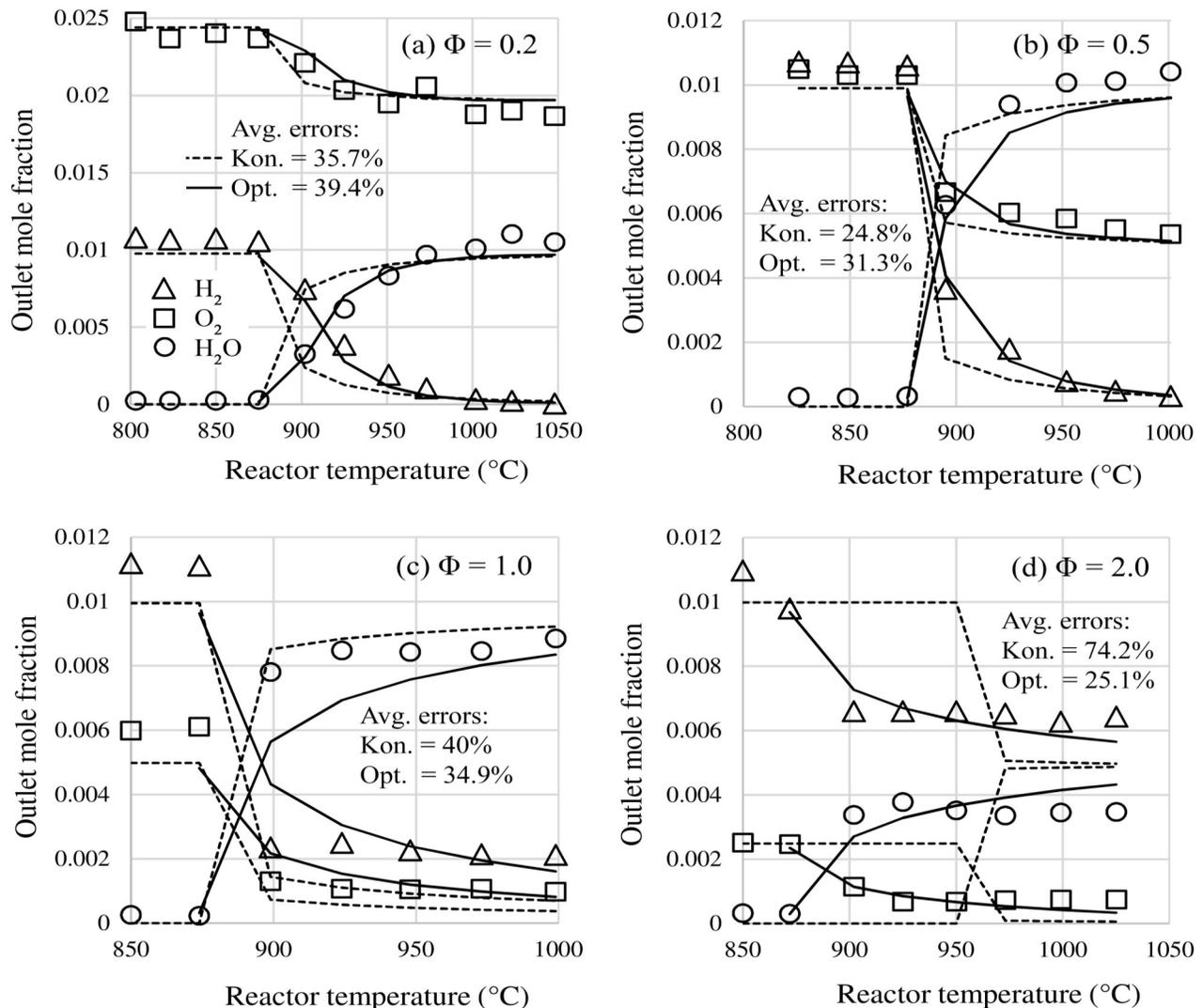


Figure 2. Predicted and experimental profile of species mole fractions vs. JSR temperature and symbols for experimental data (Cong and Dagaut, 2009).

Optimized Model Performance

Perfectly-Stirred Reactor

Using the optimized and original models, the 34 operating conditions were simulated and the outlet concentrations were compared with experimental data from Cong and Dagaut, (2009), as shown in Figure 2.

Konnov's mechanism (2008) showed good agreement with experimental data at lean condition, but by increasing the fuel-air equivalence ratio (Φ), it deviated from the experimental data points (dashed lines). It could be seen that the deviations are much higher at conditions of combustion extinction (Figure

2d). However, the optimized mechanism has been strengthened in this circumstance.

Ignition Delay Time

The validity of the optimized mechanism was assessed and approved using ignition delay time. Through available datasets for H_2 ignition in literature, Herzler *et al.* (2009) conducted a comprehensive shock-tube study of $H_2/CH_4/C_2H_6$ blends with argon diluent at different pressures. They reported 67 data points for pure hydrogen in lean condition ($\Phi = 0.5$ and 1.0). In addition to the already mentioned data, 62 data points in rich conditions ($\Phi = 4.0$) from Naumann *et al.* (2011) study were used. These test runs were re-simulated using

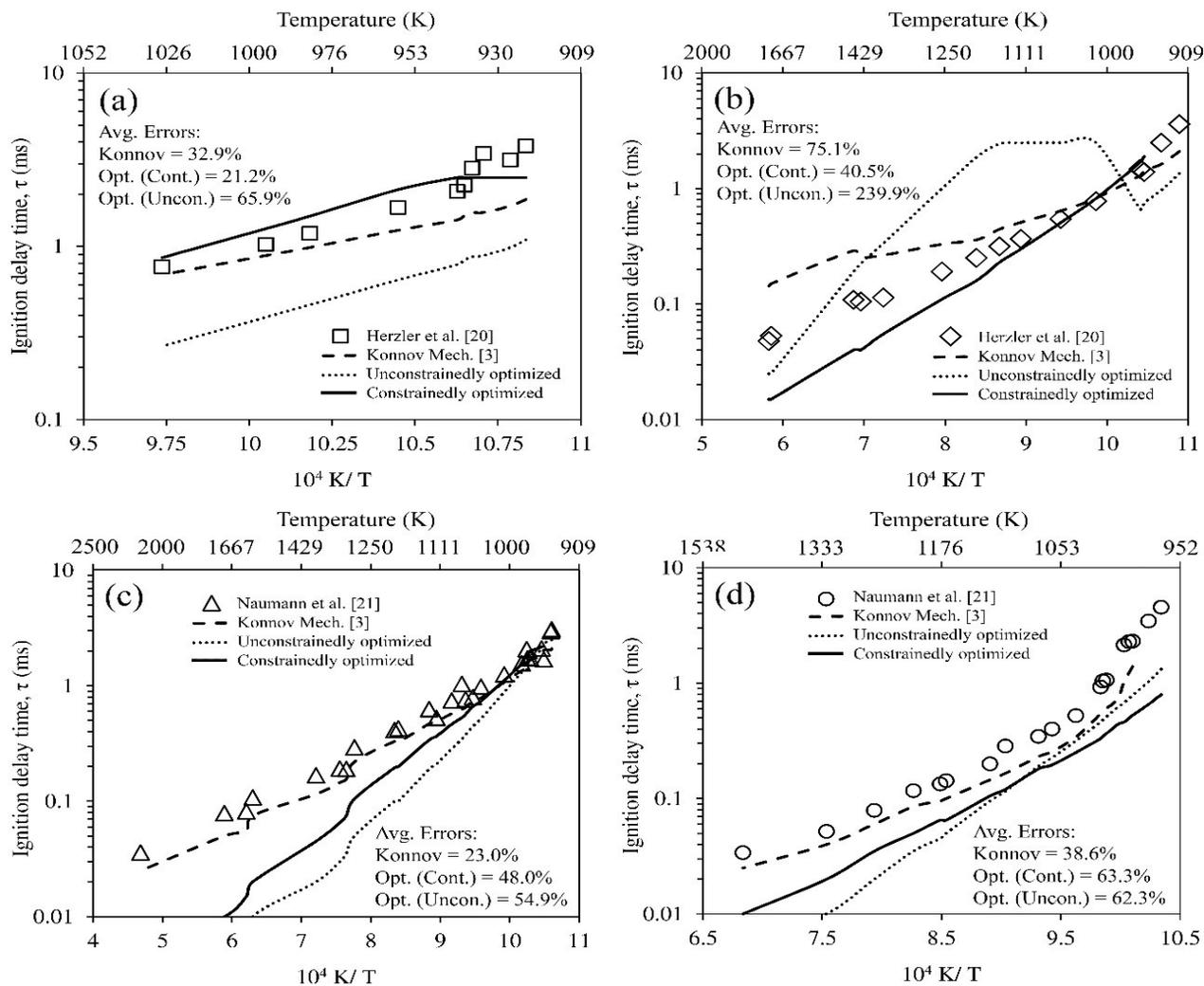


Figure 3. Comparison of experimental and calculated profile of ignition delay times vs. temperature at $P = 1$ atm; (a) $\Phi = 0.5$; (b) $\Phi = 1.0$; (c) $\Phi = 4.0$; and (d) $\Phi = 4.0$ and $P = 4$ atm.

Konnov’s mechanism (2008), unconstrained and constrained optimized mechanisms as well as the calculated ignition delay times (time of maximum OH*) were compared against the experimental data. Figure 3 illustrates the comparison of calculated and experimental ignition delay times.

As clearly seen, the unconstrained optimized mechanism showed very large deviations in the predicted ignition delay times, based on the results obtained from the experimental and two other mechanisms. Therefore, its validity was rejected. Though, the rate constants from the unconstrained optimization constituted a mathematical solution that predicted the best results of

the JSR outlet, they resulted to large deviations in the other combustion phenomena (eg. Harris *et al.*, 2000; Kéromnès *et al.*, 2013).

The constrained optimized mechanism produced better prediction when compared to Konnov’s mechanism (2008) at lean and stoichiometric conditions (Figures 3a, 3b). But at rich condition ($\Phi = 4.0$), its performance decreased especially at higher pressure (Figures 3c, 3d). These deviations may have originated from the referenced data for optimization. As shown in Figure 3, only 8 of 34 JSR data points of Cong and Dagaut, (2009) were related to rich condition ($\Phi = 2.0$).

Therefore, large errors of predicted ignition delay time at such an extrapolated condition was not so unexpected.

CONCLUSION

GA was applied to optimize the rate constants of Konnov's mechanism (2008) for H₂/O₂ combustion. The performance of optimization algorithm and final results have been discussed in details. It was shown that the constrained optimized mechanism has higher performance in comparison with Konnov's mechanism (2008) in both JSR and ignition delay time experiments.

Since the JSR experiments are easier to use and analyze, the recent data of H₂ combustion within JSR was used as the only reference data points in this study. It was shown that the results of this kinetic model are comparable with highly validated mechanisms (eg. Konnov's mechanism (2008)).

GA has very good potential to optimize combustion kinetic models, if sufficient experimental data is provided. Unconstrained optimization of the mechanism, resulted in mathematically optimum solution which has physically unrealistic reaction rates. The major reason for this outcome is lack of concentrations of intermediate species in the reference data points, which increased the degree of freedom of optimization. The results of this study showed that incorporating physical bounds in the optimization process as constraints is necessary. Elliott *et al.* (2003) applied bounds for each reaction from the Chemical Kinetic Database of National Institute of Sciences and Technology (NIST) and the bounds for species concentrations was used in this study that showed similar results.

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