



# Development of a new skeletal mechanism for decalin oxidation under engine relevant conditions



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## ABSTRACT

Being one typical cyclo-alkane class component of commercial jet and diesel fuels, decalin has two fused six-membered rings and so far few studies of decalin were accessible to its oxidation mechanism. So that this study aims to propose a skeletal mechanism of decalin oxidation that facilitates the formulating of surrogate fuels applicable in power device like engines. In this study, a skeletal mechanism of decalin oxidation was developed based on the decoupling methodology. It contains 42 species and 163 reactions, in which a simplified mechanism for the oxidation of  $C_2$ – $C_{10}$  is used to model the oxidation of heavy hydrocarbons for the prediction of the ignition characteristics, while the mechanism of  $H_2/CO/C_1$  was considered in details for the prediction of intermediate species concentrations. Among all intermediate combustion products,  $C_2H_2$  is designated as the most important soot precursor and will be used to predict soot tendency in the future study. The present skeletal mechanism was extensively validated against available fundamental experiments in regard of decalin oxidation under engine relevant conditions, wherein the temperature and pressure were relatively high. The computational results indicated that the predicted ignition delay in shock tubes and species concentrations in jet stirred reactors as well as in laminar premixed flames agree reasonably well with the measurements.

## 1. Introduction

To address the challenge on energy crisis and environment pollution, new generation fuel or surrogate fuel are broadly investigated via both digital engineering approaches and experimental test. Decalin is a typical bicyclic alkane with two fused six-membered rings and it is a crucial component in commercial jet and diesel fuels [1]. It was also proved to be significant in the new generation of fuels derived from oil shale and oil sand [2]. Thus it has attracted much attention on engine cooling due to its effective endothermic fuel capability [2,3]. As a result, decalin has been regarded as a typical cyclo-alkane class component in the development of jet fuel and diesel fuel surrogates [4,5] and their kinetic model [6]. In internal combustion (IC) engine, the processing of fuel oxidation plays significant role on auto-ignition, combustion and products formation. However, only quite a few experimental data on the oxidation of decalin can be found in the existing literature compared with the decalin pyrolysis, as listed in Tables 1 and 2. In fact, the processing of decalin oxidation is extreme complex. According to Dagaut et al. [7], H-abstraction reactions from decalin result in the formation of three  $C_{10}H_{17}$  radicals, and successive isomerization and decomposition reactions can form up to eight different decalyl radicals as shown in Fig. 1, which is just the first stage of the chemical

reaction. As such, very few researchers worked on the detailed kinetic modeling of decalin oxidation as shown in Table 3, not to mention the development of a skeletal mechanism for decalin oxidation. The detailed mechanism proposed by Dagaut et al. [7] are able to accurately capture the ignition characteristics as well as species concentrations in a jet stirred reactor. However, it is unrealistic to be used in multi-dimensional simulations of engine combustion since it has a large number of reactions (11000). Zeng et al. [8] proposed a mechanism with fewer reactions (3218), but it cannot reflect the low temperature regime and the negative-temperature-coefficient (NTC) behaviour which is pretty significant in engine combustion. To the best of our knowledge, so far no any skeletal mechanism for decalin oxidation has been developed.

In this study, a skeletal mechanism was developed for decalin oxidation containing 42 species and 163 reactions based on the decoupling methodology. Validations of the present skeletal mechanism were conducted by comparing with the experimental data on decalin oxidation under engine relevant conditions including ignition delay times in a shock tube and species concentrations in a jet stirred reactor and laminar premixed flames.

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**Table 1**  
Previous experiment on the pyrolysis of decalin.

Refs.	T (K)	P (atm)	Product distribution?
[9]	973–1223	0.5 (partial)	Yes
[10]	1093	1.78	Yes
[11]	1053, 1073	1	Yes
[12]	973–1123	1	Yes
[13]	1083	1, 2	Yes
[14]	1083	1	Yes
[15]	770–1020	1	Yes
[16]	300–1450	10–8	Yes
[17]	1015–1193	1	Yes
[18]	698–748	23–75	Yes
[3]	700–810	20–100	Yes
[19]	1083	3.95	Yes
[20]	920–1500	0.04, 0.2, 1	Yes

## 2. Model development

In this study, a decoupling methodology is used, which describes the chemistries for the oxidation of larger molecules  $C_2$ – $C_{10}$  and smaller ones  $H_2/CO/C_1$  respectively. In this methodology, a simplified mechanism for the oxidation of  $C_2$ – $C_{10}$  is used to model the oxidation of heavy hydrocarbons, while the mechanism of  $H_2/CO/C_1$  was considered in details. A detailed introduction of the decoupling methodology for the establishment of chemical kinetic mechanisms has been conducted by Chang et al. [27]. The reaction paths of the decalin skeletal mechanism developed in this study are summarized in Fig. 2. As can be seen, the mechanism is constructed by integrating the  $C_4$ – $C_{10}$  skeletal sub-mechanism with a  $C_2$ – $C_3$  reduced mechanism and a detailed mechanism of  $H_2/CO/C_1$ .

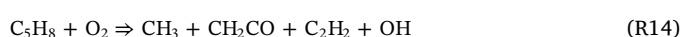
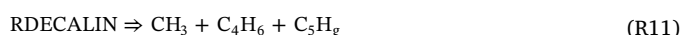
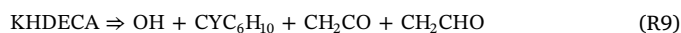
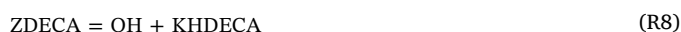
Previous investigations [28–30] have proved that the ignition delay time of heavy hydrocarbons could be successfully predicted over a wide range of conditions by using an extremely simplified  $C_4$ – $C_n$  model. Besides, the fact that quite few reactions in the simplified  $C_4$ – $C_n$  model will also lead to not very huge optimization workload to match the ignition delay time in the development of the kinetic mechanism. In this study, for each class of  $C_4$ – $C_{10}$  species, only one representative species is retained to reduce the number of species without considering different isomers in the mechanism. Based on the sensitivity analysis for the detailed decalin mechanism developed by Dagaut et al. [7], the isomers of large hydrocarbons are lumped. In Fig. 2, the structure of  $C_4$ – $C_{10}$  skeletal sub-mechanism can be seen intuitively.

In low-temperature reactions, the negative-temperature-coefficient (NTC) behaviour is a well-acknowledged aspect of straight-chain alkanes [31,32], branched-chain alkanes [33,34] and some jet fuels [35,36]. According to Agosta et al. [23], similar NTC behaviour for decalin oxidation is also noted in terms of carbon monoxide production. Following the H-atom abstraction reactions (R1–R4), an  $O_2$  is added to RDECALIN to produce RDECOO (R5), which then undergoes isomerization to form QDECOOH (R6). One more  $O_2$  is added to QDECOOH so as to produce ZDECA (R7). Furthermore, an OH is released from ZDECA to produce KHDECA (R8), after that KHDECA decomposes

**Table 2**  
Previous experiment on the oxidation of decalin.

Refs.	T (K)	P (atm)	$\Phi$	Type of experiment	Type of data
[21]	1060–1290	0.6–1.5	0.1, 0.2	Reflected shock wave	Ignition delay time
[22]	993–1305	9–48	0.5, 1.0	Reflected shock wave	Ignition delay time
[23]	600–800	8	0.3	Flow reactor	CO production
[17]	1060–1113	1	0.65–0.93	Flow reactor	Product speciation
[24]	626–731	8	0.3	Flow reactor	CO production
[25]	750–950	5–17	0.25	Motored engine	Product speciation
[26]	769–1202	11.7–51.2	0.5, 1.0, 2.0	Reflected shock wave	Ignition delay time
[8]	500–2200	0.0395	0.7, 1.0, 1.8	SVU-PIMS	Product speciation

to form  $CYC_6H_{10}$  via reaction (R9). In high-temperature reactions, RDECALIN undergoes direct ring opening reactions to form  $C_5H_8$  and  $C_4H_6$ , and simplified to (R11) by reactions lumping, then further to produce smaller species via reactions (R12–R14).



The  $C_4$ – $C_{10}$  skeletal sub-mechanism and the detailed  $H_2/CO/C_1$  mechanism are connected by the transition reactions which are obtained from a  $C_2$ – $C_3$  reduced mechanism developed by Patel et al. [37] due to its small size (10 species and 28 reactions) and satisfactory performance [38,39]. Further enhancement of the  $C_2$ – $C_3$  reduced mechanism was performed by including the important reactions for the prediction of laminar flame speed, which were identified using sensitivity analysis of the detailed mechanism from Metcalfe et al. [40].

The detailed  $H_2/CO/C_1$  mechanism is obtained from Li et al. [41] for oxidation reaction of  $CO/H_2O/H_2/O_2$ ,  $CH_2O$ , and  $CH_3OH$ , which was further developed for methanol oxidation [42] and  $H_2O_2$  kinetic model [43]. The application of the detailed  $H_2/CO/C_1$  mechanism in this study is due to the following reasons. First of all, investigations from [44–46] have revealed that most of the heat release is from the conversion of carbon monoxide (CO) to carbon dioxide ( $CO_2$ ) during the oxidation of hydrocarbons. Because the heat release process has dramatic influence on engine combustion and emissions, it is significant to predict the oxidation of CO with this decalin skeletal mechanism. Moreover, in order to better understand the sources of hydrocarbon (HC) emission in some advanced engine combustion strategies, such as homogeneous charge compression ignition (HCCI), partially premixed combustion (PPC) and reactivity controlled compression ignition (RC-CI), the formation and oxidation of light hydrocarbons should be considered in detail. The detailed  $H_2/CO/C_1$  mechanism has been proved to be able to accurately predict the formation and oxidation of small hydrocarbons under engine relevant conditions so as to predict the final HC emission. Finally, the mechanism for  $H_2/CO/C_1$  is much more

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