Decane Oxidation in a Shock Tube

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ABSTRACT: The ignition delay of *n*-decane and oxygen diluted in argon was investigated for a series of mixtures ranging from 0.49 to 1.5% decane and 4.16 to 23.25% O₂ diluted in argon. The temperature range was 1239–1616 K and the pressure range was 1.82–10.0 atm. All experiments were performed in a heated shock-tube. An overall ignition delay equation was deduced for 144 experiments: $\tau = 10^{-12} \exp(+34240/RT) |C_{10}H_{22}|^{0.60} |O_2|^{-1.305} |Ar|^{0.08}$ s. Product distribution from preignition periods were measured. Detailed simulation schemes available in the literature were checked and a corrected model is proposed that fits well our experiments. © 2006 Wiley Periodicals, Inc. Int J Chem Kinet 38: 703–713, 2006

INTRODUCTION

Normal decane ($C_{10}H_{22}$) is one of the most obvious ingredients of diesel fuel although its concentration in diesel oil distillates does not exceed 3%. It was also defined as one of three ingredients (the others being methyl naphthalene and normal heptane) and sometimes as one of two ingredients (the other being toluene) that their blend should be used to simulate diesel fuel.

A short list of experimental and numerical studies of *n*-decane combustion has been reported lately [1-9] and these include Dagaut et al. [1], Westbrook and coworkers [2], Warnatz and coworkers [3], Battin-Leclerc and coworkers [4,5], Lindstedt and Maurice [6], Dryer and coworkers [7], Peters and coworkers [8], and Wilson and coworkers [9]. In these studies, oxidation mechanisms were validated against different types of *n*-decane experiments in the gas phase, mainly jet stirred reactors and premixed flame propagation measurements. Ignition delay times were reported at a minimum.

Ignition delay measurements were performed in a heated shock tube by Adomeit and coworkers [12] for *n*-decane/air mixtures at 12 and 50 bar pressure and temperature range (T_5) of 700–1300 K. The purpose of these experiments was mainly to describe a twostep oxidation process at high- and low-temperature regions. They found a negative temperature trend in their ignition experiments. The number of experiments, variety of the test-mixtures, and pressure conditions were not sufficient for statistical analysis. These results were used for decane oxidation modeling by three groups [3,7,8]. One group [7] validated their *n*-decane autoignition mechanism against these experimental data in the temperature range 1000-1300 K. It should be noticed that in the lower part of the temperature interval (1000–1150 K), the model overpredicted the ignition delay time. Another group [8] proposed an oxidation mechanism, which fitted well the experimental data at temperatures 700-1250 K with good prediction of the temperature's negative trend region. In all the modeling studies, the models were compared directly against individual experiments rather than an overall experimental expression (not supplied up to now), which applies to a broader range of pressures, temperatures, and compositions. Such a correlation was proposed by Lifshitz [10] more than



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30 years ago and since then it has been extensively used. It should be mentioned the work of Davidson and coworkers [11] where the authors try to correlate four sets of stoichiometric mixtures for four different normal alkanes (propane, butane, heptane, and decane), with oxygen diluted in argon and statistically regress them together using Lifshitz's [10] formula to obtain a general correlation for autoignition of *n*-alkanes. The authors proposed a single expression for all four alkanes' ignition delay time with an activation energy of 46 kcal/mol. They used their own experiments for decane ignition, which were performed with only one stoichiometric test-mixture of decane– O_2 –Ar under a narrow range of temperature and pressure levels.

The purpose of the present study is to provide a set of experiments for *n*-decane that can be presented with an overall ignition delay correlation (Lifshitz formula) in order to compare it to other hydrocarbons on similar basis. The second purpose is to present a mechanism that will fit the experimental data. As it is well known, the single pulse shock tube experiments are the closest possible representation of the PSR (perfect stirred reactor) concept. Any other kind of combustion kinetic experiment such as flame measurements and even plug flow reactors includes some hard-to-define nonchemical parameters such as flow, heat transfer, and wall reactions.

Some researchers claim that a mechanism is better if it fits as many experimental systems as possible. In the end, they represent a mechanism that is a compromise among the different available results. The question is "What is the purpose of such a mechanism?" Our idea is to obtain the best simulation of a PSR experiment in order to obtain the best description of PSR conditions.

EXPERIMENTAL

Ignition delay experiments were performed behind reflected shock waves in a heated single pulse shock tube. This instrument serves as a heater in the millisecond range, where the walls remain at constant temperature (100°C in our case).

Ignition delay times, as measured in this shock-tube study, are the time intervals between the rapid rise of the pressure due to the shock arrival and the onset of the pressure due to the ignition.

The shock tube is made of a 4 m long stainless steel tube. The driven section is 2.5 m long. Mylar diaphragms of different gauges were burst to generate the shock wave. Maximal ignition delay and cooling times behind the reflected shocks were 2 ms. The aerodynamic cooling achieved was $\sim 10^6$ K/s.

The sampling section of 0.25 long contains three Kistler 603A piezoelectric transducers. Two transducers 0.20 m apart measure the shock velocity from which the temperature is calculated. A third piezoelectric gauge, located on the end plate, records the ignition delay time. The pressure outputs are fed to digital oscilloscopes that record 12-bit traces of 4098 points, each at 1 μ s intervals.

The reflected shock temperatures were calculated using standard conservation equations and the ideal gas equation of state assuming frozen chemistry.

Thermodynamic data for all the species were taken from Burcat's compilation [13]. The temperature uncertainty error was ± 20 K.

The materials for these experiments were n-decane product of Aldrich 99+% pure. The oxygen and argon of pure quality (98%) were purchased from Oxygen Stores, Haifa. The materials were used as it is without further purification. Twenty liter heated glass bulbs were used to store the mixtures. The mixtures were left for more than 24 h to mix. These mixtures served as stock for the individual experiments. The analysis of postshock gases was performed by taking samples of the gas into preevacuated glass bulbs of ~100 cc and analyzed on a Hewlett-Packard 5900 model gas chromatograph equipped with a flame ionization detector and containing a 6 feet long PORAPACK N column and a PACKARD 427 gas chromatograph with a PORAPACK O column. A Perkin-Elmer/Nelson Analytical PC Integrator was connected to the flame ionization detector of both instruments. The gas inlets and the mixture in the bulb were heated during the analyses with the PACKARD 427 instrument.

RESULTS

The oxidation of decane was investigated by measuring the ignition delay of *n*-decane–oxygen–argon blends in a single pulse shock tube. End plate pressure traces were used to measure the ignition delay as defined above. Mixtures of 0.5-1.5 mol% decane and 4.2-23 mol% oxygen diluted in argon were used at pressures between 1.8 and 9.4 atm. Table I is a list of the mixtures and conditions used in the experiments as well as representative shocks from each mixture. In Fig. 1, a least square statistical analysis of all the 144 experiments is presented in order for them to satisfy the Lifshitz equation [10] of the ignition delay time

$$\tau(\mathbf{s}) = A \exp\left(+\frac{E}{RT}\right) [C_{10}H_{22}]^a [O_2]^b [Ar]^a$$

Mixture No.	Symbol	[Dec] (%)	$\left[O_{2}\right] (\%)$	Num Exp. ^a	Num Stat. ^b	Experiment No.	P_1 (Torr)	P_5 (atm)	T_5 (K)	au (µs)
1	Δ	1.5	23.25	31	20	8	51	2.70	1448	60
						15	70	3.24	1362	118
						29	70	3.82	1478	36
2	0	0.52	8.4	19	17	35	251	7.25	1384	101
						40	240	6.25	1282	314
						43	71	2.57	1532	66
						49	70	1.82	1282	657
3	+	0.82	11.0	20	18	55	241	7.01	1270	299
						59	240	9.29	1473	35
						66	70	3.13	1592	41
						68	72	2.37	1352	258
5	\diamond	0.49	7.5	20	17	96	241	7.57	1432	82
						99	239	8.09	1492	45
						106	70	1.81	1291	667
						111	69	2.28	1471	120
6	∇	0.74	12.7	20	15	114	242	6.63	1239	321
						117	241	9.11	1463	30
						124	72	2.31	1343	263
						128	70	3.17	1616	21
7	•	0.81	4.16	20	17	135	242	8.2	1427	216
						139	241	10.0	1594	70
						145	71	2.84	1560	180
						150	68	2.28	1418	641
8	0	0.75	7.40	20	18	157	241	8.86	1481	60
						159	241	6.60	1268	496
						163	70	2.71	1523	110
						167	70	1.96	1284	792
9		0.78	17.6	27	22	177	70	2.73	1452	58
						182	70	2.03	1237	490
						197	70	3.08	1535	25

Table I Representative Experiments of *n*-Decane–Oxygen–Argon Mixtures

^{*a*} The actual number of experiments performed.

^b The number of experiments used for the statistical analysis. The rest were discarded.

The overall ignition delay of decane based on a $\sigma = 2$ spread of 144 experiments is $\tau = 10^{-12\pm0.2}$ $\exp(+34240/RT)[C_{10}H_{22}]^{0.60\pm0.06}[O_2]^{-1.305\pm0.042}$ $[Ar]^{0.08\pm0.05}$ s. The overall ignition delay of decane based on a $\sigma = 3$ spread of 168 experiments is $\tau = 10^{-11.9\pm0.4} \exp(+34600/RT)[C_{10}H_{22}]^{0.66\pm0.09}$ $[O_2]^{-1.33\pm0.06}[Ar]^{0.055\pm0.068}$ s.

Some experiments were conducted so that the quenching rarefaction wave arrived before ignition occurred. These experiments were called "preignition" shocks. The postshock preignition samples of gas were gathered and analyzed for products in a gas chromatograph. The postshock products detected were CO₂, CH₄, C₂H₄, C₂H₆, C₃H₆, C₄H₆, 1-C₄H₈, 1-C₅H₁₀, 1-C₆H₁₂, 1-C₇H₁₄, and 1-C₈H₁₆. No higher products than C₈ were detected except for decane itself. In Figs. 2 and 3, the different intermediate oxidation ingredients found in the preignition gas chromatographic analysis are shown as concentration of specie at temperature *T* normalized by the initial decane concentration ($[Specie]_T/[C_{10}H_{22}]_0$) versus 1/T.

MODELING AND CALCULATIONS

The modeling of *n*-decane worth mentioning is the Westbrook's [2], Battin-Leclerc's [4,5], Lindstedt's [6], and Wilson's [9]. We have tried most of these models one way or another and found that all of them do not fit our experiments and give calculations that are far lower from the main experimental line and/or have a steeper activation energy. Of special interest is the work of Battin-Leclerc and coworkers [4,5], which was achieved using an automatic mechanism generator Exgas [3]. Some researchers envision such computer programs as achieving final/absolute answers to kinetic problems.



Figure 1 Ignition delay times of 144 experiments with the notation from Table I. The statistically reduced least squares satisfy the equation $\tau = 10^{-12} \exp(+34240/RT)$ $[C_{10}H_{22}]^{0.60}[O_2]^{-1.305}[Ar]^{0.08}$ s.

The problem with this automatic reaction generator is that it gives too much attention to all the possibilities of radical reactions whether they exist or not. This causes the models to be blown up beyond proportions to thousands of reactions that cannot be followed by humans because of the human limitations. The consequences are obvious.

The proposed mechanism was built on previous proposed schemes. To keep the mechanism in manageable conditions, we had to reduce the number of possible isomer products, and to adjust some of the rates so that the final scheme will not only predict the experimental Lifshitz equation of *n*-decane but also fit the experimental concentration of products (Figs. 2 and 3). Equations were chosen for rate change following sensitivity analysis tests that were conducted at a multitude of temperature and conditions.

Our kinetic scheme contains 433 reactions and 69 species. The first 270 reactions are from *n*-pentane oxidation model [15], which is basically Westbrook's scheme [16,17]. We eliminated 2- and 3-pentyl radicals and 2-pentene from this mechanism as explained above. Only 1-pentyl and 1-pentene remained in our *n*-decane mechanism. In the following reactions of $C-C_2$ submechanism, the parameters from the new GRI (ver. 3.0) are used:

$$H + O_2 \rightleftharpoons O + OH,$$

$$k = 2.5 \times 10^{16} T^{-0.67} \exp\left(-\frac{17040}{RT}\right)$$

$$C_{2}H_{3} + O_{2} \rightleftharpoons CH_{2}O + CHO,$$

$$k = 4.58 \times 10^{16} T^{-1.39} \exp\left(-\frac{1015}{RT}\right)$$

$$C_{2}H_{4} + CH_{3} \rightleftharpoons C_{2}H_{2} + CH_{4},$$

$$k = 2.27 \times 10^{5} T^{2.0} \exp\left(-\frac{9200}{RT}\right)$$

The second part of the decane-ignition scheme includes reactions of hydrocarbons from C_6 to C_{22} that are presented in Table II.

As initiation reactions in our kinetic scheme, we have considered the following steps of *n*-decane pyrolysis:

$$\begin{split} C_{10}H_{22} \rightleftharpoons C_2H_5 + C_8H_{17} \\ C_{10}H_{22} \rightleftharpoons C_3H_7 + C_7H_{15} \\ C_{10}H_{22} \rightleftharpoons C_4H_9 + C_6H_{13} \\ C_{10}H_{22} \rightleftharpoons C_5H_{11} + C_5H_{11} \end{split}$$

with kinetic parameters close to Bikas and Peters [8]: activation energy (81–82 kcal/mol) and preexponential factor multiplied by 1.5–2.5 values. It should be noticed that the activation energy in Battin-Leclerc and coworkers [4,5] had higher values \sim 83–87 kcal/mol whereas Lindstedt and Maurice [6] used a much smaller value for the decane pyrolysis stages, in the range of \sim 68 kcal/mol. The initiation also includes the formation of three different decyl radicals (reactions 5–7 in Table II).

The kinetic parameters of H-abstraction reactions, followed by decyl radical formation, are proposed in our mechanism mainly by analogy for *n*-heptane oxidation used by Chakir et al. [18]. Some corrections are made only on the preexponential factor (see Table II) while the activation energy and *n*-parameter for temperature remained without changes.

As explained in [18], the *n*-heptane possesses four distinguishable H-atom sites; therefore, four heptyl radicals are produced by H atom abstraction. The rate constants of these reactions depend on the nature of the H-abstraction site and the number of the hydrogen atoms present in the site. As for *n*-pentane H-abstraction reactions [19a], the kinetic data used in this case were derived from recommendations of Tamura [19b].

In [18], for n-C₇H₁₆ + H \rightleftharpoons 1-C₇H₁₅ + H₂, $A = 2.81 \times 10^7$ is given. For n-C₇H₁₆ + H \rightleftharpoons 2-C₇H₁₅ + H₂, $A = 0.91 \times 10^7$ is given. The same is for 3-C₇H₁₅, and for 4-C₇H₁₅, $A = 4.5 \times 10^6$ is given. These values do not follow exactly the rules of Tamura, because they were fit for the [18] model. H abstraction by other



Figure 2 Product distribution of CH_4 , C_2H_4 , C_3H_6 , and C_4H_8 species vs. calculated parameters from our model represented by the solid inverted triangles and the least square line. Concentration of specie at temperature *T* normalized by the initial decane concentration. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

radicals in their paper (CH₃, HO₂, C₂H₅) follow exactly Tamura's recommendations (*A*-factor according to the number of the H-atom in every abstraction site).

There are five different decyl-radicals, which may be formed in *n*-decane oxidation, although in our work we consider as explained above only three of them, which we considered more important $(n-C_{10}H_{21}, 2-C_{10}H_{21})$, and $3-C_{10}H_{21}$).

In our mechanism, the same "*n*" and " E_a " were used as in [18], because the H-abstraction site for C₁₀H₂₂ and C₇H₁₆ are similar, but the preexponential factor *A* for 1-C₁₀H₂₁ was slightly changed ($A = 3.5 \times 10^7$). Taking into account that the 4- and 5-decyls, that were omitted, may increase the quantity of 2- and 3-decyls, the *A*factor for 2- and 3-decyl was doubled (0.91×10^7) × 2. As a result $A = 1.9 \times 10^7$. The parameters for reactions of H-abstraction with H-radical are taken from Battin-Leclerc and coworkers [4,5]. There are great differences in kinetic parameters for H-abstraction reactions with CH₃-radical in the articles considered for *n*-decane oxidation [4,5,8] and we used preexponential factors in our scheme from [18], multiplying by 2. The preexponential factor for H-abstraction reaction by HO₂-radical with the formation of *n*-decyl is taken from [4,5] whereas the values for 2-decyl and 3-decyl formation are very different in references [4,5] and [8], namely -4×10^{12} and -10^{14} , respectively. We used *A*-factors for these reactions for corresponding radicals by analogy to *n*-heptane [18].

The rate constants for isomerization of decylradicals are taken according to [18], which originate



Figure 3 Product distribution of C_5H_{10} , C_6H_{12} , C_7H_{14} , and C_8H_{16} species vs. calculated parameters from our model represented by the solid inverted triangles and the least square line. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

in Westbrook's work, and are very close to those of Battin-Leclerc and coworkers [4,5].

In our scheme, it is proposed that decenes are formed in reaction of decyl radicals with O_2 followed by HO_2 formation. We take into consideration, in order to reduce redundancy, only two decenes with double bond on the first and second C-atoms. Kinetic parameters for decene formation are taken by analogy for corresponding heptyl reactions [18] with the correction of the A-factor. The decenes are consumed by thermal decomposition into smaller radicals and olefins and by additive reactions with O and OH, which are followed by rupture of C–C bonds. The rates of these reactions for both groups are taken from [18] for 1,2- and 3-heptenes. H-abstraction reactions from decenes by H, O, OH, and CH₃-radicals are proposed to lead to only one alkenyl radical (C₁₀H₁₉) for both decenes (C₁₀H₂₀ and C₁₀H₂₀-2). This radical is supposed to decompose in analogy to C₇H₁₃ in the *n*-heptane oxidation process. The kinetic parameters for its decomposition into two smaller parts are taken from the corresponding reactions of C₇H₁₃ [18,20].

As we do not take into consideration decyl-radicals on carbons 4 and 5 in our modeling, we suppress formation of some intermediate species resulting from these radicals. To compensate the formation of some olefins, which appear in our oxidation experiments before ignition at temperature 1020–1070 K, we

Reaction	$A ({\rm mol/cm^3})$	N	$E_{\rm a}$ (kcal/mol)	Remarks
$\overline{C_{10}H_{22}} \rightleftharpoons C_2H_5 + C_8H_{17}$	6.50E+16	0.0	82.0	*b, see text
$C_{10}H_{22} \rightleftharpoons C_3H_7 + C_7H_{15}$	8.50E+16	0.0	81.0	*b, see text
$C_{10}H_{22} \rightleftharpoons C_4H_9 + C_6H_{13}$	4.50E+16	0.0	82.0	*b, see text
$C_{10}H_{22} \rightleftharpoons C_5H_{11} + C_5H_{11}$	4.3E+16	0.0	81.0	*b, see text
$C_{10}H_{22} \rightleftharpoons C_{10}H_{21} + H$	1.00E+15	0.0	100.0	*a-139
$C_{10}H_{22} \rightleftharpoons C_{10}H_{21}-2+H$	1.00E+15	0.0	100.0	*a-140
$C_{10}H_{22} \rightleftharpoons C_{10}H_{21}-3 + H$	1.00E+15	0.0	100.0	*a-141
$C_{10}H_{22} + H \rightleftharpoons C_{10}H_{21} + H_2$	3.51E+07	2.0	7.7	[3]
$C_{10}H_{22} + H \rightleftharpoons C_{10}H_{21} - 2 + H_2$	1.91E+07	2.0	5.0	[3]
$C_{10}H_{22} + H \rightleftharpoons C_{10}H_{21} - 3 + H_2$	1.91E+07	2.0	5.0	[3]
$C_{10}H_{22} + O \rightleftharpoons C_{10}H_{21} + OH$	7.60E+06	2.4	1.59	*a-12, A*3
$C_{10}H_{22} + O \rightleftharpoons C_{10}H_{21} - 2 + OH$	6.40E+05	2.5	5.0	*a-13
$C_{10}H_{22} + O \rightleftharpoons C_{10}H_{21} - 3 + OH$	6.40E+05	2.5	5.0	*a-14
$C_{10}H_{22} + OH \rightleftharpoons C_{10}H_{21} + H_2O$	1.05E + 10	0.97	1.59	*a-16
$C_{10}H_{22} + OH \rightleftharpoons C_{10}H_{21} - 2 + H_2O$	4.70E + 07	1.61	0.0	*a-17
$C_{10}H_{22} + OH \rightleftharpoons C_{10}H_{21} - 3 + H_2O$	4.70E + 07	1.61	0.0	*a-18
$C_{10}H_{22} + CH_3 \rightleftharpoons C_{10}H_{21} + CH_4$	6.00E+12	0.0	11.6	*a-20, A*2
$C_{10}H_{22} + CH_3 \rightleftharpoons C_{10}H_{21} - 2 + CH_4$	3.20E+12	0.0	9.5	*a-21, A*2
$C_{10}H_{22} + CH_3 \rightleftharpoons C_{10}H_{21} - 3 + CH_4$	3.20E+12	0.0	9.5	*a-22, A*2
$C_{10}H_{22} + HO_2 \rightleftharpoons C_{10}H_{21} + H_2O_2$	1.12E+13	0.0	19.4	*a-24
$C_{10}H_{22} + HO_2 \rightleftharpoons C_{10}H_{21} - 2 + H_2O_2$	6.80E+12	0.0	17.0	*a-25
$C_{10}H_{22} + HO_2 \rightleftharpoons C_{10}H_{21} - 3 + H_2O_2$	6.80E+12	0.0	17.0	*a-26
$C_{10}H_{22} + O_2 \rightleftharpoons C_{10}H_{21} + HO_2$	2.51E+13	0.0	49.0	[3]
$C_{10}H_{22} + O_2 \rightleftharpoons C_{10}H_{21} - 2 + HO_2$	3.98E+13	0.0	47.6	Est, see text
$C_{10}H_{22} + O_2 \rightleftharpoons C_{10}H_{21} - 3 + HO_2$	4.00E+13	0.0	47.6	Est
$C_{10}H_{21} \rightleftharpoons C_2H_4 + C_8H_{17}$	7.52E+12	0.0	28.8	[3], A/3
$C_{10}H_{21}-2 \rightleftharpoons C_3H_6 + C_7H_{15}$	1.00E + 13	0.0	28.3	[3], A/3
$C_{10}H_{21}-3 \rightleftharpoons C_4H_8 + C_6H_{13}$	1.00E + 13	0.0	29.1	[3], A/3
$C_{10}H_{21}-3 \rightleftharpoons C_9H_{18} + CH_3$	8.0 E+12	0.0	33.0	[3], A/3
$C_{10}H_{21} \rightleftharpoons C_{10}H_{20} + H$	1.00E + 13	0.0	40.4	*a-57
$C_{10}H_{21}-2 \rightleftharpoons C_{10}H_{20} + H$	1.00E + 13	0.0	40.4	*a-58
$C_{10}H_{21}-2 \rightleftharpoons C_{10}H_{20}-2 + H$	1.00E+13	0.0	40.4	*a-59
$C_{10}H_{21}-3 \rightleftharpoons C_{10}H_{20}-2 + H$	1.00E+13	0.0	40.4	*a-60
$C_{10}H_{21} \rightleftharpoons C_{10}H_{21}$ -2	2.00E+11	0.0	11.1	*a-63
$C_{10}H_{21} \rightleftharpoons C_{10}H_{21}-3$	2.00E+11	0.0	18.1	*a-64
$C_{10}H_{21}-2 \rightleftharpoons C_{10}H_{21}-3$	2.00E+11	0.0	20.0	*a-66
$C_{10}H_{21} + O_2 \rightleftharpoons C_{10}H_{20} + HO_2$	2.00E+12	0.0	2.0	*a-67, A*2
$C_{10}H_{21}-2+O_2 \rightleftharpoons C_{10}H_{20}+HO_2$	2.00E+12	0.0	4.5	*a-68, A*2
$C_{10}H_{21}-2+O_2 \rightleftharpoons C_{10}H_{20}-2+HO_2$	3.00E+12	0.0	4.25	*a-69, A*1.5
$C_{10}H_{21}-3+O_2 \rightleftharpoons C_{10}H_{20}-2+HO_2$	3.00E+12	0.0	4.25	*a-70, A*1.5
$C_{10}H_{20} \rightleftharpoons C_7H_{15} + C_3H_5$	2.52E+16	0.0	71.1	*a-73
$C_{10}H_{20}-2 \rightleftharpoons C_6H_{13} + C_4H_7$	1.60E + 16	0.0	69.3	*a-74
$C_{10}H_{20} + H \rightleftharpoons C_{10}H_{19} + H_2$	8.00E+13	0.0	3.4	*a-77, see text
$C_{10}H_{20} + O \rightleftharpoons C_{10}H_{19} + OH$	4.00E+13	0.0	4.0	*a-80
$C_{10}H_{20} + OH \rightleftharpoons C_{10}H_{19} + H_2O$	2.00E+13	0.0	2.6	*a-83
$C_{10}H_{20} + CH_3 \rightleftharpoons C_{10}H_{19} + CH_4$	2.00E+11	0.0	6.8	*a-86
$C_{10}H_{20} + HO_2 \rightleftharpoons C_{10}H_{19} + H_2O_2$	2.50E+12	0.0	0.0	*a-89, A/2
$C_{10}H_{20} + O \rightleftharpoons C_{2}H_{3} + C_{8}H_{16} + OH$	2.82E + 13	0.0	5.2	*a-92, see text
$C_{10}H_{20} + O \rightleftharpoons C_{3}H_{5} + C_{7}H_{14} + OH$	2.82E+13	0.0	5.2	^a-93
$C_{10}H_{20} + O \rightleftharpoons C_4H_7 + C_6H_{12} + OH$	2.82E + 13	0.0	5.2	^a-94 * 02
$C_{10}H_{20} + O \rightleftharpoons C_5H_9 + C_5H_{10} + OH$	2.82E+13	0.0	5.2	^a-93
$C_{10}H_{20} + O \rightleftharpoons C_4H_8 + C_6H_{11} + OH$	2.82E+13	0.0	5.2	*a-93
$C_{10}H_{20} + O \rightleftharpoons C_{3}H_{6} + C_{7}H_{13} + OH$	2.82E+13	0.0	5.2	^a-93 *- 05
$C_{10}H_{20} + O \rightleftharpoons C_2H_4 + C_8H_{15} + OH$	5.00E + 13	0.0	/.8	^a-95
$C_{10}H_{20} + OH \rightleftharpoons C_{3}H_{5} + C_{7}H_{14} + H_{2}O$	1.29E+09	1.25	0.7	^a-102

Table IIKinetic Scheme of C_{10} -C6 Used in Our Mechanism

710 OLCHANSKI AND BURCAT

Table II	Continued

Reaction	$A \text{ (mol/cm}^3)$	Ν	$E_{\rm a}$ (kcal/mol)	Remarks
$C_{10}H_{20} + OH \rightleftharpoons C_4H_7 + C_6H_{12} + H_2O$	1.29E+09	1.25	0.7	*a-103
$C_{10}H_{20} + OH \rightleftharpoons C_5H_9 + C_5H_{10} + H_2O$	1.29E+09	1.05	0.7	*a-104
$C_{10}H_{20} + OH \rightleftharpoons C_2H_3 + C_8H_{16} + H_2O$	1.29E+09	1.25	0.7	*a-101
$C_{10}H_{20} + OH \rightleftharpoons C_4H_8 + C_6H_{11} + H_2O$	1.29E+09	1.25	0.7	*a-103
$C_{10}H_{20} + OH \rightleftharpoons C_3H_6 + C_7H_{13} + H_2O$	1.29E+09	1.25	0.7	*a-103
$C_{10}H_{20} + OH \rightleftharpoons C_2H_4 + C_8H_{15} + H_2O$	4.27E+09	1.05	1.81	*a-107
$C_{10}H_{20}-2+H \rightleftharpoons C_{10}H_{19}+H_2$	0.80E+14	0.0	3.4	*a-78, see text
$C_{10}H_{20}-2 + O \rightleftharpoons C_{10}H_{19} + OH$	4.00E+13	0.0	4.0	*a-81
$C_{10}H_{20}-2 + OH \rightleftharpoons C_{10}H_{19} + H_2O$	2.00E+13	0.0	2.6	*a-84
$C_{10}H_{20}-2+CH_3 \rightleftharpoons C_{10}H_{19}+CH_4$	2.00E+11	0.0	6.8	*a-87
$C_{10}H_{20}-2+HO_2 \rightleftharpoons C_{10}H_{19}+H_2O_2$	2.50E+12	0.0	0.0	*a-90
$C_{10}H_{20}-2+O \rightleftharpoons C_6H_{11}+C_4H_8+OH$	2.82E+13	0.0	5.2	*a-96
$C_{10}H_{20}-2+O \rightleftharpoons C_7H_{13}+C_3H_6+OH$	2.82E+13	0.0	5.2	*a-97
$C_{10}H_{20}-2+O \rightleftharpoons C_5H_{10}+C_5H_9+OH$	2.82E+13	0.0	5.2	*a-97
$C_{10}H_{20}-2+OH \rightleftharpoons C_6H_{11}+C_4H_8+H_2O$	1.16E+09	1.25	0.7	*a-105
$C_{10}H_{20}-2 + OH \rightleftharpoons C_7H_{13} + C_3H_6 + H_2O$	1.16E+09	1.25	0.7	*a-106
$C_{10}H_{20}-2 + OH \rightleftharpoons C_5H_{10} + C_5H_9 + H_2O$	1.16E+09	1.25	0.7	*a-105
$C_{10}H_{22} + H \rightarrow H_2 + C_5H_{11} + C_5H_{10}$	2.1E+06	2.4	4.47	*d-260
$C_{10}H_{22} + H \rightarrow H_2 + C_2H_5 + C_8H_{16}$	2.1E+06	2.4	4.47	*d-246
$C_{10}H_{22} + OH \rightarrow H_2O + C_5H_{11} + C_5H_{10}$	3.0E+06	2.0	-1.312	*d-262
$C_{10}H_{22} + OH \rightarrow H_2O + C_2H_5 + C_8H_{16}$	3.0E+06	2.0	-1.312	*d-250
$C_{10}H_{22} + O \rightarrow OH + C_5H_{11} + C_5H_{10}$	2.5E+05	2.6	1.91	*d-261
$C_{10}H_{22} + O \rightarrow OH + C_2H_5 + C_8H_{16}$	2.5E+05	2.6	1.91	*d-248
$C_{10}H_{22} + HO_2 \rightarrow H_2O_2 + C_5H_{11} + C_5H_{10}$	0.2E + 04	2.6	13.9	*d-264
$C_{10}H_{22} + HO_2 \rightarrow H_2O_2 + C_2H_5 + C_8H_{16}$	0.16E+04	2.6	13.9	*d-255
$C_{10}H_{22} + O_2 \rightarrow HO_2 + C_5H_{11} + C_5H_{10}$	1.0E+13	0.0	47.6	*d-263, A/4
$C_{10}H_{22} + O_2 \rightarrow HO_2 + C_2H_5 + C_8H_{16}$	0.5E+13	0.0	47.6	*d-253, A/2
$C_{10}H_{22} + C_3H_5 \rightarrow C_3H_6 + C_2H_5 + C_8H_{16}$	7.8E+01	3.3	18.16	*d-266
$C_{10}H_{22} + C_3H_5 \rightarrow C_3H_6 + C_5H_{11} + C_5H_{10}$	7.8E+01	3.3	18.16	*d-266
$C_{10}H_{20}-2+O \rightleftharpoons C_3H_5+C_7H_{14}+OH$	2.82E+13	0.0	5.2	*a-97
$C_{10}H_{19} \rightleftharpoons C_3H_5 + C_7H_{14}$	2.52E+13	0.0	30.0	*a-110
$C_{10}H_{19} \rightleftharpoons C_4H_6 + C_6H_{13}$	1.0E+13	0.0	32.0	*a-112
$C_9H_{18} \rightleftharpoons C_4H_9 + C_5H_9$	2.0E+16	0.0	68.0	
$C_9H_{18} + H \rightleftharpoons C_9H_{17} + H_2$	8.0E+13	0.0	3.4	*a-77
$C_9H_{18} + O \rightleftharpoons C_9H_{17} + OH$	4.00E+13	0.0	4.0	*a-80
$C_9H_{18} + OH \rightleftharpoons C_9H_{17} + H_2O$	2.00E+13	0.0	2.6	*a-83
$C_9H_{18} + CH_3 \rightleftharpoons C_9H_{17} + CH_4$	2.00E+11	0.0	6.8	*a-86
$C_9H_{18} + HO_2 \rightleftharpoons C_9H_{17} + H_2O_2$	2.50E+12	0.0	0.0	*a-89, A/2
$C_9H_{18} + O \rightleftharpoons C_2H_3 + C_7H_{14} + OH$	2.82E+13	0.0	5.2	*a-92
$C_9H_{18} + O \rightleftharpoons C_3H_5 + C_6H_{12} + OH$	2.82E+13	0.0	5.2	*a-93
$C_9H_{18} + O \rightleftharpoons C_4H_7 + C_5H_{10} + OH$	2.82E+13	0.0	5.2	*a-94
$C_9H_{18} + O \rightleftharpoons C_5H_9 + C_4H_8 + OH$	2.82E+13	0.0	5.2	*a-93
$C_9H_{18} + OH \rightleftharpoons C_3H_5 + C_6H_{12} + H_2O$	1.29E + 09	1.25	0.7	*a-102
$C_9H_{18} + OH \rightleftharpoons C_4H_7 + C_5H_{10} + H_2O$	1.29E + 09	1.25	0.7	*a-103
$C_9H_{18} + OH \rightleftharpoons C_5H_9 + C_4H_8 + H_2O$	1.29E + 09	1.25	0.7	*a-102
$C_9H_{18} + OH \rightleftharpoons C_2H_3 + C_7H_{14} + H_2O$	1.29E + 09	1.25	0.7	*a-101
$C_9H_{17} \rightleftharpoons C_4H_7 + C_5H_{10}$	2.0E+12	0.0	30.0	*a-138
$C_9H_{17} \rightleftharpoons C_3H_5 + C_6H_{12}$	2.0E+12	0.0	30.0	*a-138
$C_9H_{17} \rightleftharpoons C_2H_3 + C_7H_{14}$	2.0E+12	0.0	30.0	*a-138
$C_8H_{17} \rightleftharpoons C_2H_4 + C_6H_{13}$	2.52E+13	0.0	28.8	[3]
$C_8H_{17} + O_2 \rightleftharpoons C_8H_{16} + HO_2$	1.00E+12	0.0	2.0	*a-67
$C_8H_{17} \rightleftharpoons C_8H_{16} + H$	1.00E+13	0.0	40.4	*a-57
$C_8H_{16} \rightleftharpoons C_3H_5 + C_5H_{11}$	2E+16	0.0	71.0	$*d-260$ to $1-C_6H_{12}$
$C_8H_{16} \rightleftharpoons C_4H_8 + C_4H_8$	4E+14	0.0	57.0	*d-210
$C_8H_{16} + H \rightarrow C_5H_{10} + C_2H_4 + CH_3$	7.23E+12	0.0	1.302	*d-212

Continued

Table II Continue	b

Reaction	$A ({\rm mol/cm}^3)$	Ν	Ea (kcal/mol)	Remarks
$C_8H_{16} + H \rightarrow H_2 + C_4H_6 + C_4H_9$	1.15E+05	2.5	2.49	*d-214
$\mathrm{C_8H_{16}+O} \rightarrow \mathrm{OH} + \mathrm{C_3H_6} + \mathrm{C_5H_9}$	4.76E + 04	2.71	2.11	*d-220
$\mathrm{C_8H_{16}+O} \rightarrow \mathrm{OH} + \mathrm{C_2H_3} + \mathrm{C_6H_{12}}$	1.3E + 06	2.4	4.47	*d-216
$C_8H_{16} + OH \rightarrow H_2O + C_4H_6 + C_4H_9$	2.08E + 06	2.0	-0.3	*d-222
$C_8H_{15} \rightleftharpoons C_2H_3 + C_6H_{12}$	2.5E+12	0.0	30.0	*a-138, A/2
$C_8H_{15} \rightleftharpoons C_3H_5 + C_5H_{10}$	2.0E+12	0.0	30.0	*a-138, A/2
$C_7H_{14} + OH \rightleftharpoons C_7H_{13} + H_2O$	2.0E+13	0.0	2.6	[19]-88
$C_7H_{14} + H \rightleftharpoons C_7H_{13} + H_2$	8.0E+13	0.0	3.4	[19]-82
$C_7H_{14} + CH_3 \rightleftharpoons C_7H_{13} + CH_4$	2.0E+11	0.0	6.8	[19]-91
$C_7H_{14} + OH \rightleftharpoons C_6H_{13} + CH_2O$	1.0E+11	0.0	0.0	*a-135
$C_7H_{14} + OH \rightleftharpoons C_5H_{11} + CH_3CHO$	1.0E+11	0.0	0.0	*a-136
$C_7H_{14} \rightleftharpoons C_3H_5 + C_4H_9$	2.52E+15	0.0	71.1	[18]-73, A/10
$C_7H_{14} + O \rightleftharpoons C_7H_{13} + OH$	4.00E+13	0.0	4.0	[19]-85
$C_7H_{14} \rightleftharpoons C_3H_7 + C_4H_7$	1.60E+15	0.0	69.3	[18]-74, A/10
$C_7H_{14} + HO_2 \rightleftharpoons C_7H_{13} + H_2O_2$	1.0E+12	0.0	0.0	[18], A/5
$C_7H_{14} + O \rightleftharpoons C_2H_3 + C_5H_{10} + OH$	2.8E+13	0.0	5.2	[19]-97
$C_7H_{14} + O \rightleftharpoons C_3H_5 + C_4H_8 + OH$	2.8E+13	0.0	5.2	[19]-98
$C_7H_{14} + O \rightleftharpoons C_4H_7 + C_3H_6 + OH$	2.8E+13	0.0	5.2	[19]-99
$C_7H_{14} + O \rightleftharpoons C_5H_9 + C_2H_4 + OH$	5.0E+13	0.0	7.85	[19]-100
$C_7H_{14} + OH \rightleftharpoons C_2H_3 + C_5H_{10} + H_2O$	6.5E+09	1.25	0.7	[19]-106
$C_7H_{14} + OH \rightleftharpoons C_3H_5 + C_4H_8 + H_2O$	1.5E+09	1.25	0.7	[19]-107
$C_7H_{14} + OH \rightleftharpoons C_4H_7 + C_3H_6 + H_2O$	1.29E+09	1.25	0.7	[19]-108
$C_7H_{14} + OH \rightleftharpoons C_5H_9 + C_2H_4 + H_2O$	4.27E+09	1.05	1.81	[19]-109
$C_7H_{15} \rightleftharpoons C_3H_6 + C_4H_9$	1.60E+13	0.0	28.3	[18]-53
$C_7H_{15} \rightleftharpoons C_2H_4 + C_5H_{11}$	2.52E+13	0.0	28.8	[4]
$C_7H_{15} + O_2 \rightleftharpoons C_7H_{14} + HO_2$	1.0E + 12	0.0	2.0	[19]-130
$C_7H_{15} \rightleftharpoons C_7H_{14} + H$	1.0E+13	0.0	40.4	[18]-57
$C_7H_{13} \rightleftharpoons C_3H_5 + C_4H_8$	2.5E+13	0.0	30.0	[18]-110
$C_7H_{13} \rightleftharpoons C_4H_6 + C_3H_7$	1.0E+13	0.0	32.0	[18]-112
$C_6H_{13} \rightleftharpoons C_6H_{12} + H$	1.0E+13	0.0	38.11	[18]-113
$C_6H_{13} + O_2 \rightleftharpoons C_6H_{12} + HO_2$	1.0E+12	0.0	2.0	[8]-313
$C_6H_{12} + OH \rightleftharpoons C_6H_{11} + H_2O$	2.0E+13	0.0	2.6	[18]-124
$C_6H_{12} + H \rightleftharpoons C_6H_{11} + H_2$	8.0E+13	0.0	3.4	[18]-122
$C_6H_{12} + CH_3 \rightleftharpoons C_6H_{11} + CH_4$	2.0E+11	0.0	6.8	[18]-123
$C_6H_{12} + OH \rightleftharpoons C_5H_{11} + CH_2O$	1.0E+11	0.0	0.0	[18]-135
$C_6H_{12} + OH \rightleftharpoons C_4H_9 + CH_3CHO$	1.0E+11	0.0	0.0	[18]-136
$C_6H_{12} \rightleftharpoons C_3H_6 + C_3H_6$	1.0E+13	0.0	56.80	[18]-121, A/5
$C_6H_{12} + O \rightleftharpoons C_3H_5 + C_3H_6 + OH$	2.80E+13	0.0	5.2	[8]-307
$C_6H_{12} + O \rightleftharpoons C_6H_{11} + OH$	4.00E + 13	0.0	4.0	[18]-123
$C_6H_{12} \rightleftharpoons C_3H_7 + C_3H_5$	2.52E + 16	0.0	71.1	[8]-302
$C_6H_{12} + HO_2 \rightleftharpoons C_6H_{11} + H_2O_2$	1.0E + 11	0.0	17.0	[18]-126
$C_6H_{12} + O \rightleftharpoons C_2H_3 + C_4H_8 + OH$	2.8E+13	0.0	5.2	[8]-308
$C_6H_{12} + O \rightleftharpoons C_4H_7 + C_2H_4 + OH$	5.0E+13	0.0	7.85	[8]-306
$C_6H_{12} + O \rightleftharpoons CHO + C_5H_{11}$	1.0E + 11	0.0	0.0	[18]-130
$C_6H_{12} + O \rightleftharpoons CH_3 + CO + C_4H_0$	1.0E + 11	0.0	0.0	[18]-131
$C_6H_{12} + OH \rightleftharpoons C_2H_3 + C_4H_8 + H_2O$	6.5E+09	1.25	0.7	[18]-132
$C_{4}H_{12} + OH \Rightarrow C_{2}H_{5} + C_{4}H_{6} + H_{2}O$	1.5E+0.9	1.25	0.7	[18]-133 A/4
$C_6H_{12} + OH \rightleftharpoons C_4H_7 + C_2H_4 + H_2O$	2.15E + 10	1.05	1.81	[18]-134
$C_6H_{12} \rightleftharpoons C_4H_0 + C_2H_4$	1.50E + 12	0.0	28.8	[4], A/10
$C_6H_{11} \rightleftharpoons C_3H_5 + C_3H_6$	5.0E + 12	0.0	30.0	[18]-137 A/10
$C_{2}H_{11} \rightleftharpoons C_{2}H_{5} + C_{4}H_{2}$	5.0E + 12 5.0E+11	0.0	32.0	[18]-138 A/10
c_{0}	5.06711	0.0	52.0	[10]-130, A/10

*a: in analogy to reaction number written in ref. [18].

*b: in analogy to reaction number written in ref. [8].

*c: in analogy to reaction number written in ref. [4,5].

*d: in analogy to reaction number written in ref. [20].



Figure 4 Comparison of experimental data with different mechanisms taken from the literature. (1) Our model; (2) Battin-Leclerc's (Exgas) model, see text; (3) Lindstedt and Maurice + GRI model; (4) Lindstedt and Maurice and Westbrook's model with changes of three of Westbrook's parameters. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

have included several semiempirical reactions into our mechanism, proposed earlier for *n*-heptane [20]. In these reactions, the decane-molecule reacts with radicals H, OH, and HO₂, which abstract H from alkane, and then the alkenyl-radical breaks into an olefin and a radical. Kinetic parameters for these semiempirical reactions are taken by analogy to *n*-heptane transformation through 3,4-heptyl [21].

Earlier proposed schemes are compared with our experimental data as shown in Fig. 4.

We used three mechanisms to validate our experimental data: Battin-Leclerc's scheme [4,5], Lindstedt and Maurice scheme [6], and our mechanism described above. All the mechanisms were calculated using the same thermodynamic database [13].

In Battin-Leclerc's automatic scheme [5], we eliminated all reactions where peroxy-radicals or compounds (including keto-peroxy) were formed, and several hundreds reactions connected with different radical isomerizations. We did that because these compounds exist only at low-temperature cool flame conditions but do not exist at our experimental conditions. In the compared mechanism, 500 reactions remained from the original of 1700+ reactions. This simulation is shown as line 2 on Fig. 4.

In Lindstedt–Maurice scheme [6], all the reactions with H-abstraction and formation of five decyl radicals, decane, and decyl pyrolysis and decyl isomerization were kept, according to $[6]^*$. The reaction of C₆ and C₇ were taken from their previous work on *n*-heptane combustion [20]. These reactions were combined with the C_3 - C_5 submechanism of our scheme with corresponding necessary changes in the A-parameter dimensions. The oxidation of small hydrocarbons $(C-C_2)$ was presented in two variants: the first was GRI (Fig. 4, line 3) and the second was Westbrook's original scheme, with changes in three reaction parameters as described in our mechanism (Fig. 4, line 4). As it can be seen in Fig. 4, the line 1 representing our model fits very well the experiments of ignition delay time. Lindstedt and Maurice scheme with $C-C_2$ from Westbrook [16,17] (Fig. 4, line 4) is parallel slightly below the experimental data and our model line. Although the difference is relatively small for ignition delay time experiments, at low temperatures we get large differences with Lindstedt-Maurice scheme in oxidation intermediate product species; thus, the concentration of small hydrocarbons is by 1-2 orders larger than the experimental data. Our mechanism fits sufficiently well the experimental data for oxidation products, as shown in Figs. 2 and 3.

In Fig. 5, we present a comparison of our model and the experimental ignition delay equation as a function



[C10H22], mol fraction

Figure 5 Our calculated model compared with the overall experimental ignition delay equation. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

^{*}In the works of Lindstedt and Maurice [6,19], there is a question about the dimensions of the A-parameter reported. They use one value for their own reactions, but the reactions taken from other papers are given as they appear in the original work, not according to the dimensions listed in the tables. We have used the reactions listed by Lindstedt and Maurice with their dimensions, thus, we multiplied by 10^3 to adjust them to our dimensions.

of τ , the ignition delay versus the fuel concentration. Here, we get a good estimation of the lean and the rich limits of combustion of *n*-decane and we are reminded again that the Lifshitz equation cannot be used outside the experimental window, but the modeling scheme will show us the correct behavior. The correct width of the U-shaped line can be seen only with a full mechanism like the one we used and any attempt to reduce the mechanism means a narrower U [15].

CONCLUSION

An experimental study of ignition of *n*-decane was presented and compared with a number of proposed kinetic mechanisms found in the literature. None of the models fitted well our findings, and none of the experimental studies from the literature could be compared with ours because of differences of presentation. In order to fit a mechanism to our experiments, many changes in individual rates were necessary. Of special disappointment was the Exgas automatic model that turned out to be the least fitting to our experiments.

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