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REACTION MECHANISM FOR THE OXIDATION OF ALLENE AND PROPYNE

Abstract. The study of detailed chemistry of allene and propyne in hydrocarbon combustion are very important, because they are precursors of propargyl radical (H_2CCCH). Propargyl radical plays a main role in formation of first aromatic molecules, benzene, which it is start to growth polyaromatic hydrocarbons (PAHs), and soot formation.

This paper focuses on the development a reaction kinetic sub-mechanism for the oxidation of allene and propyne which is included in the reaction data of the base of the DLR. The detailed chemistry of allene and propyne is a part of earlier published C_2-mechanism with polyaromatic hydrocarbons (PAHs) formation. The sub-mechanism of C_3H_4 reaction was analyzed on the basis of published studies. Experimental data of ignition delay times and laminar flame speed have been used for validation and improvement of general oxidation reaction paths. In the results, the mechanism was adopted 6 reactions; the rate constants for 7 reactions at the high- (T>1500K) and low-temperatures (T<1500K) ignition were modified. The rate coefficients for reactions $C_3H_4 + H = H_2CCCH + H_2$, $C_3H_4 + H = CH_3 + C_2H_2$ and $C_3H_4 + HO_2 = H_2CCCH + H_2O_2$ have evaluated with statistical treatment. Modified model shows to accurately reproduce the ignition delay times and laminar flame speed of both allene and propyne mixtures at p_5=2-10 bar, T_5=1100-1840 K and ϕ=0.5-2.0 and laminar flame speed at T_0=298K, p=1 bar, ϕ=0.6-1.8.

Keywords: modeling, mechanism, allene, propyne, oxidation.

Introduction. Polycyclic aromatic hydrocarbons (PAHs) and soot particles are among the priority pollutants, as they have carcinogenic activity and are dangerous for human health. In this connection, the scientific interests to investigation the kinetic mechanism of PAHs and soot formation have not weakened in recent decades [1-3].

The study of detailed chemistry of allene and propyne in hydrocarbon combustion and pyrolysis are very important, because they are precursors of propargyl radical (H_2CCCH). It is now well established as experimentally and as theoretically that propargyl radical is important radical, which is a critical intermediate on the formation of the first aromatic ring, PAHs, and soot formation.

This paper aim is to develop a reaction kinetic sub-mechanism for the oxidation of allene and propyne.

C_3H_4-sub model. The detailed chemistry of allene and propyne is a part of earlier published C_2 mechanism [4] which consists of 111 species and 920 reversible elementary reactions. This mechanism has been initially validated against ignition delay data [5, 6] and laminar flame speed [7] of both allene- and propyne-oxygen-argon at pressures p_5 = 2–10 bar and for a wide range of stoichiometries ϕ = 0.5–2.0. The characteristic data of experimental flames and their uncertainties are summarized in Table 1.

Table 1 – Evaluation of uncertainty intervals for the selected shock tube experimental data

Ref.	Driven section				T_5, K		p_5, bar		φ	Dilution	t_{meas}, μs	Uncert., %
	L, m		Int. d, cm									
[5]	3.65	+5%	4.5	+5%	1200-1900	+5%	2.0-5.0	+5%	0.5-2.0	yes	+5%	45%
[6]	4.0	+5%	7.8	+5%	1000-1650		8.5-10.0	+5%	0.5-1.0	yes	+10%	45%
*Initial uncertainty is 20%.												

Numerical modelling was performed using the SENKIN (for simulation of ignition delay time) and PREMIX (for simulation of laminar flame speed, sensitivity analysis, rate of production analysis (ROPAD)) code from the CHEMKIN II package [8] and Chemical Workbench [9].

The initially validation against experimental data of ignition delay time and laminar flame speed shows that the mechanism is described the oxidation of allene and propyne (C_3H_4) the range of temperature interval 1300–1500 K, but does not describe at high- (T > 1500K) and low-temperature (T < 1300K).

First step of the improving the sub-mechanism of C_3H_4 is sensitivity analysis, which to identify the most important reactions for the development of the oxidation reaction chain. Analysis have been carried for several temperatures, as at satisfactory described (T_5 = 1381 K) and as at unsatisfactory described (T_5 = 1893 K, T_5 = 1636K, T_5 = 1226 K). For every temperature 10 major reactions, which influence to ignition delay time are shown in Figure 1. This analysis has shown that allene/propyne decomposition reaction $H_2CCCH + H (+M) = C_3H_4 (+M)$ (R403) is important reaction for low- and high-temperatures. Another the most important reactions for high temperature are H-consuming reactions: $C_3H_4 + H = H_2CCCH + H_2$ (R395) and $C_3H_4 + H = CH_3 + C_2H_2$ (R397); and to low temperatures $C_3H_4 + HO_2 = H_2CCCH + H_2O_2$ (R396) reaction.

The theoretical and experimental rate constant of reactions (R395)-(R396), which were recommended in literature from different sources [10-20] have demonstrated that these rates are different at same flame temperatures. For instance, the rate constant of Davis et al. [10] for reaction (R395) is almost 100 times faster than the corresponding rate of Miller et al. [13]. The rate coefficients for reactions

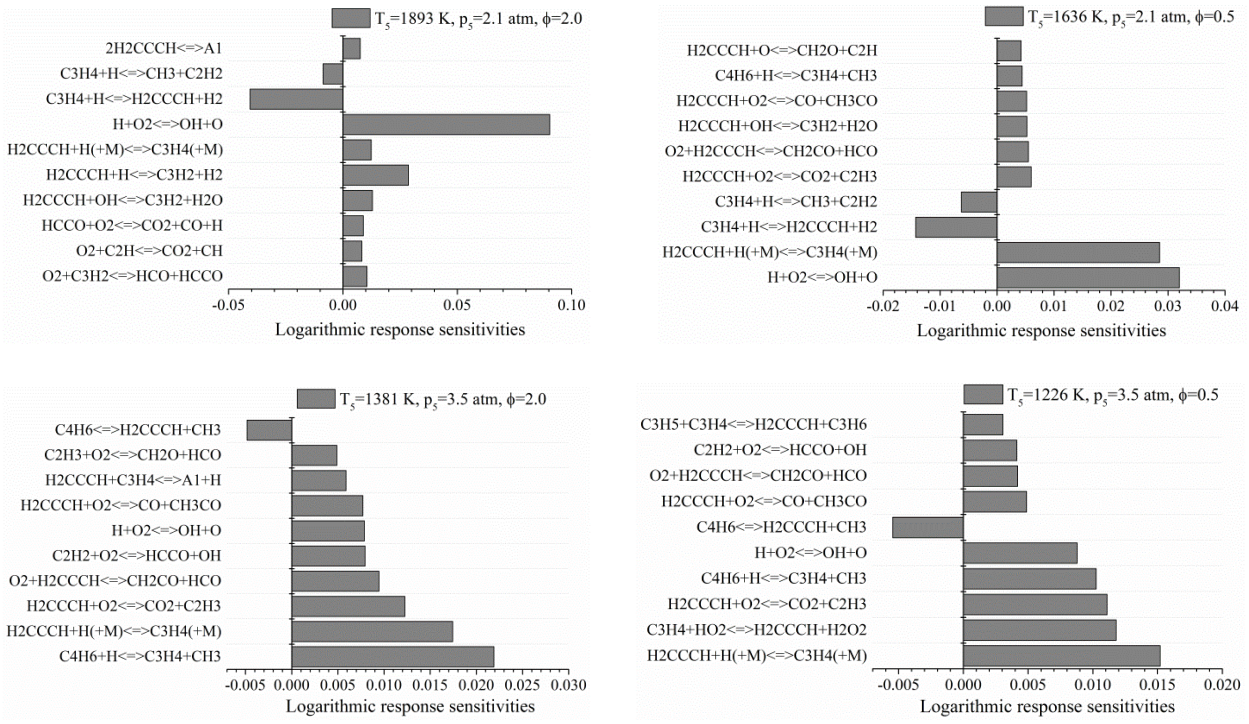

Figure 1 – Logarithmic response sensitivities computed with initial C_2 mechanism for ignition delay time

$C_3H_4 + H = H_2CCCH + H_2$ (R395), $C_3H_4 + H = CH_3 + C_2H_2$ (R397), and $C_3H_4 + HO_2 = H_2CCCH + H_2O_2$ (R396) have evaluated with statistical treatment (Figure 2). This allows the calculation of the uncertainty factor, *f(T)*, (generally not symmetric) traditionally used in chemical kinetics to determine the uncertainty level for the reaction:

$$f_u(T) = \frac{k_{upper}(T)}{k_0(T)}; \qquad f_l(T) = \frac{k_0(T)}{k_{low}(T)},$$

where k_0 is the nominal rate coefficient in the Arrhenius expression (cm^3, *mol, s, K*)

$$k(T) = AT^n \exp(-E_a/T),$$

A, n, Ea – Arrhenius parameters; k_{low} and k_{upper} are lower and upper bounds, respectively.

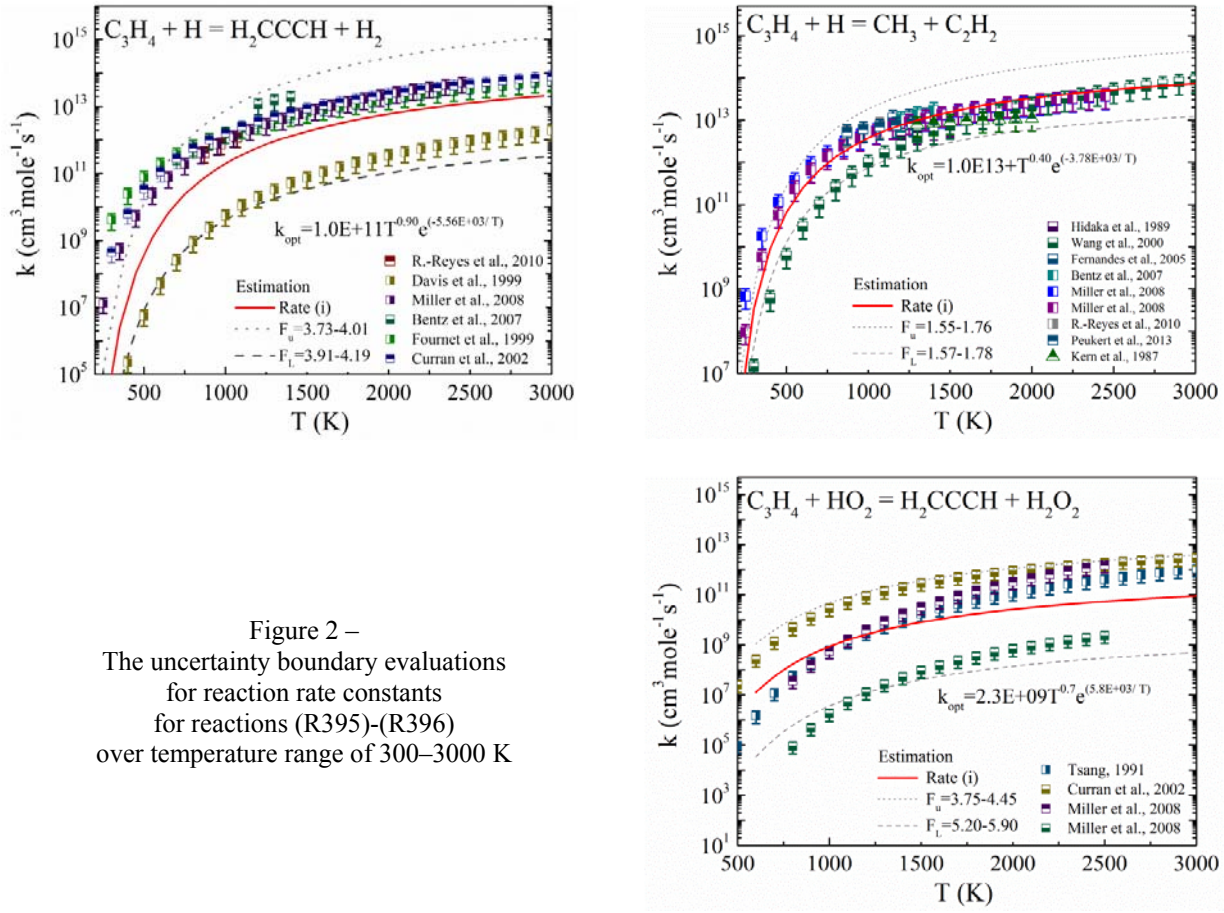

Figure 2 –
The uncertainty boundary evaluations
for reaction rate constants
for reactions (R395)-(R396)
over temperature range of 300–3000 K

To improve simulations of ignition delay times at high-temperature the reactions (R375), (R398)-(R402) were newly adopted.

The unimolecular decomposition reaction (R398) competing to reaction (R403) plays an important role at high temperature as well. The reactions of hydrogen abstraction (R399)-(R402) were added in the model, because they are important reactions for the chain propagation and active radical production. The reaction rate coefficients $k_{398} - k_{400}$ were adopted from Fournet et al. [6]; the rates of reactions k_{401} and k_{402} were added from Zhang et al. [21].

The important reaction for the chain brunching (R375) was studied by Klippenstein et al. [2] at T = 600–2000 K and p = 0.001–100 atm. The reaction rate coefficients for (R376) and (R380) were analyzed and revised. Finally, the rate coefficient values followed from [22] were prescribed to these reactions (Table 2).

Table 2 – Modifications in the DLR mechanism conducted in the present work

N	Reactions	A	n	Ea	Ref.
R375	$H_2CCCH=C_3H_2+H$	3.500E+38	-6.78	54250.0	[2]
R376	$H_2CCCH+OH=HCO+C_2H_3$	4.000E+12	0.00	0.00	[22]
R377	$H_2CCCH+H=C_3H_2+H_2$	5.000E+11	0.00	0.00	[23]
R380	$H_2CCCH+O_2=CO_2+C_2H_3$	3.010E+09	0.00	1443.0	[22]
R385	$H_2CCCH+OH=C_3H_2+H_2O$	2.000E+12	0.00	0.00	[24]
R395	$C_3H_4+H=H_2CCCH+H_2$	1.000E+12	0.90	5560.0	[Est.]
R396	$C_3H_4+HO_2=H_2CCCH+H_2O_2$	2.300E+10	0.70	5800.0	[Est.]
R397	$C_3H_4+H=CH_3+C_2H_2$	1.000E+14	0.40	3780.0	[Est.]
R398	$C_3H_4=C_2H+CH_3$	4.200E+16	0.00	50000.0	[6]
R399	$C_3H_4+OH=CH_2O+C_2H_3$	2.000E+12	0.00	100.0	[6]
R400	$C_3H_4+HO_2=C_2H_4+CO+OH$	6.000E+09	0.00	4000.0	[6]
R401	$C_3H_4+OH=HCO+C_2H_4$	1.000E+12	0.00	0.00	[21]
R402	$C_3H_4+O=CH_2O+C_2H_2$	9.000E+12	0.00	1870.0	[21]

*Est. – Rate constants were estimated in this work. The rate constants are given at 1 atm ($k(T) = AT^n \exp(-E_a/T)$) in *cm^3, mol, s, K* units.

The addition of these reactions led to the improved agreement with experimental data of ignition delay time at high-temperature. However, the simulation shows that oxidation of allene at lower-temperature should be further investigated. The principal scheme of low-temperature oxidation for allene and propyne will be developed and oxygenated compounds like C_3H_4O, $C_3H_4O_2$, C_3H_2O will be added to the model.

Final simulation with C_3H_4-sub model is shown that adopted and modified reactions reproduce accurately the ignition delay time for both of allene and propyne mixture flame at high-temperature, Figure 3.

The present kinetic model predicts the shape of the laminar flame speed curve reasonably well, but it over-predicts the experimental data at lean to stoichiometric equivalence ratios (ϕ = 0.7–1.1) (Figure 4). Based on the model, the consumption of propyne and allene in laminar premixed flame is mainly due to reaction R398.

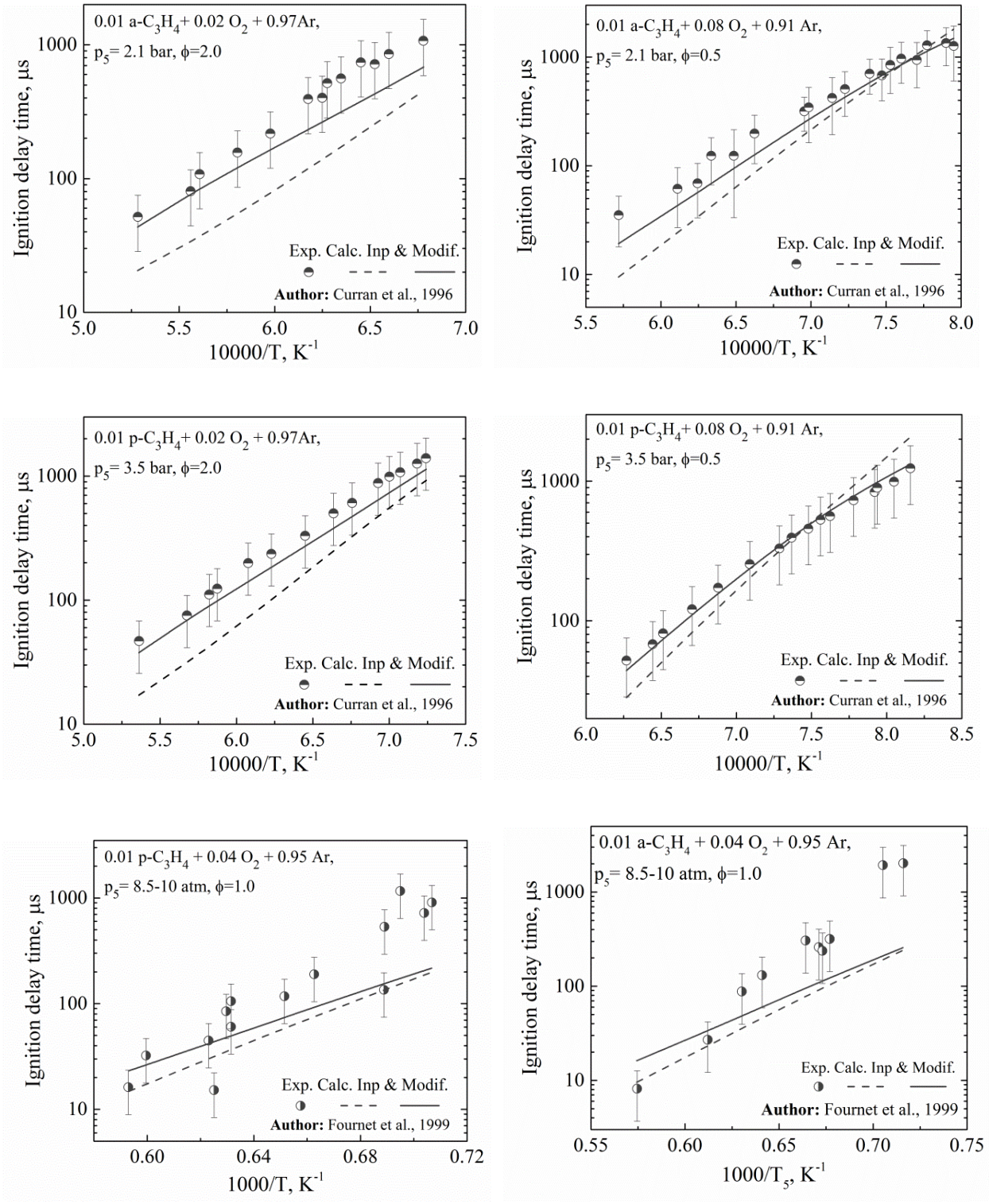

Figure 3 – Comparison between computed (dash line – initial-;
solid lines – modified- mechanism) and experimental (symbols) ignition delay times of $C_3H_4/O_2/Ar$ mixtures [5, 6]

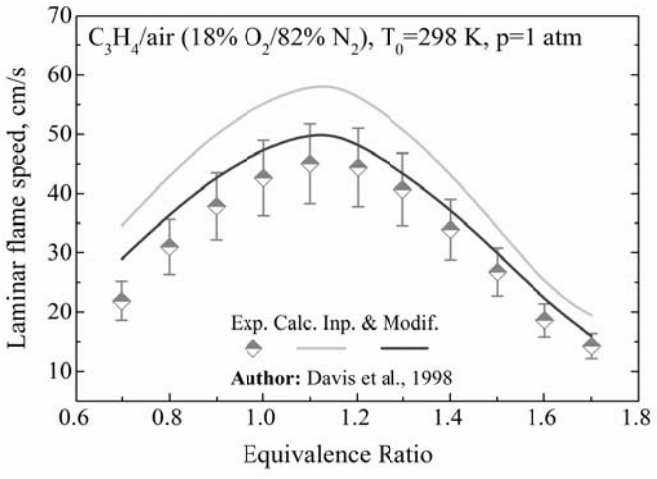

Figure 4 – Experimental (symbol) [7] and computed (line) of the laminar flame speed of C_3H_4/air flame

The complete scheme of the main reaction paths of oxidation and pyrolysis of allene and propyne at high temperature in C_3H_4-sub model are shown on the Figure 5.

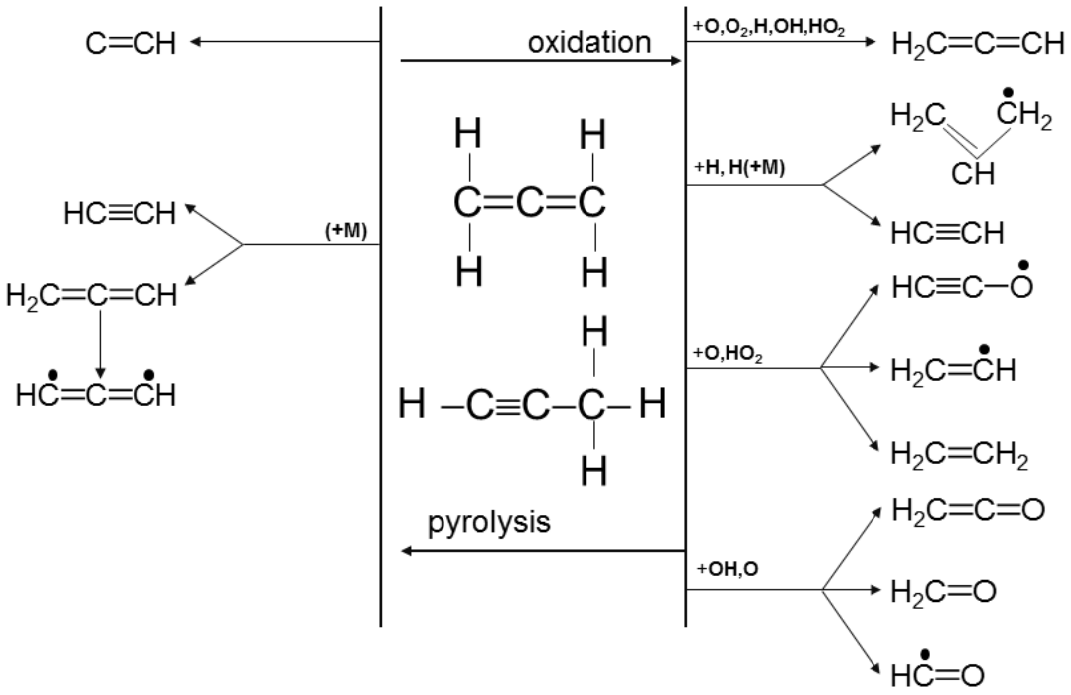

Figure 5 – The major initial stages of oxidation and pyrolysis of allene and propyne in C_3H_4-sub model

Conclusion. A detailed kinetic model was modified and verified against the experimental data of the shock-tube ignition delay and the laminar flame speed data available in the literature. It was shown that sub-mechanism of C_3H_4 predicts the allene and propyne oxidation and pyrolysis at high-temperature data reasonably well. The sensitivity analysis shows that reaction of C_3H_4=C_2H+CH_3 plays the important role in pyrolysis of allene and propyne at high temperature. A detailed kinetic C_3H_4 sub-mechanism of oxidation of allene and propyne for low-temperature will be discussed later.

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АЛЛЕН ЖӘНЕ ПРОПИННІҢ ТОТЫҒУ РЕАКЦИЯСЫНЫҢ МЕХАНИЗМІ

Аннотация. Көмірсутектер жанғанда түзілетін аллен жане пропиннің химиясын толық зерттеу өте маңызды, себебі олар пропаргил радикалының (H_2CCCH) прекурсорлары болып табылады. Пропаргил радикал, полициклді ароматты көмірсутектердің (ПЦАК) және күйе бөлшектерінің түзілуінде бастапқы рөл атқаратын бірінші ароматты молекула – бензолдың түзілуінде өте маңызды.

Осы мақалада НАО-ның реакциялық базасы негізінде аллен мен пропиннің тотығуының суб-механизмінің кинетикалық реакциясын жасауға көніл бөлінді. Аллен мен пропиннің химиясы бұрын жарияланған ПЦАК бар C_2 механизмнің бір бөлігі болып табылады. C_3H_4 суб-механизміндегі реакцияларға жарияланған зерттеу жұмыстар негізінде талдау жасалды. Тұтану уақыты және ламинарлы жалын жылдамдығының эксперименттік деректері реакция механизмін тексеру және оңтайландыру үшін пайдаланылды. Нәтижесінде, механизмге 6 реакция қосылды; төменгі ($T < 1500K$) және жоғары температурада ($T > 1500K$) тұтану уақытын сипаттау үшін 7 реакцияның жылдамдылық константасы жанартылды. $C_3H_4 + H = H_2CCCH + H_2$, $C_3H_4 + H = CH_3 + C_2H_2$ және $C_3H_4 + HO_2 = H_2CCCH + H_2O_2$ реакцияларының жылдамдылық коэффициенттері деректерді статистикалық өңдеу арқылы бағаланды. Өңделген модел аллен және пропин қоспасы үшін $p_5 = 2–10$ бар, $T_5 = 1100–1840$ К, $\phi = 0,5–2,0$ кезінде тұтану уақытың және $T_0 = 298K$, $p = 1$ bar, $\phi = 0,6–1,8$ кезіндегі ламинарлы жалынның жылдамдылығын толық сипаттайды.

Түйін сөздер: моделдеу, механизм, аллена, пропен, тотығу.

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МЕХАНИЗМ РЕАКЦИЙ ОКИСЛЕНИЯ АЛЛЕНА И ПРОПИНА

Аннотация. Изучение детальной химии аллена и пропина при горении углеводородов очень актуально, поскольку они являются прекурсорами пропаргильного радикала (H_2CCCH). Пропаргильный радикал играет основную роль в образовании первой ароматической молекулы, бензола, который дает старт росту полициклических ароматических углеводородов (ПЦАУ) и образованию сажи.

В настоящей работе основное внимание уделяется разработке реакционного кинетического суб-механизма для окисления аллена и пропина, входящего в реакционную данных базу НАЦ (DLR). Детальная химия аллена и пропина является частью ранее опубликованного механизма C_2 с образованием ПЦАУ. Суб-механизм реакции C_3H_4 был проанализирован на базе опубликованных исследований. Экспериментальные данные по временам задержек воспламенения и скоростям ламинарных пламен были использованы для тестирования и оптимизации реакционного механизма. В результате механизм был дополнен 6 реакциями; константы скоростей 7 реакций для низкотемпературного ($T < 1500K$) и высокотемпературного ($T > 1500K$) воспламенения были модифицированы. При этом коэффициенты скоростей реакций $C_3H_4 + H = H_2CCCH + H_2$, $C_3H_4 + H = CH_3 + C_2H_2$ и $C_3H_4 + HO_2 = H_2CCCH + H_2O_2$ были оценены путем статистической обработки данных. Модифицированная модель удовлетворительно воспроизводит времена задержек воспламенения для смесей аллена и пропина при $p_5 = 2$-10 бар, $T_5 = 1100–1840$ К, $\phi = 0,5–2,0$ и скорости ламинарных пламен для аллена при $T_0 = 298K$, $p = 1$ bar, $\phi = 0,6–1,8$.

Ключевые слова: моделирование, механизм, аллен, пропин, окисления.

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