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OF THE REPUBLIC OF KAZAKHSTAN

ХИМИЯ ЖӘНЕ ТЕХНОЛОГИЯ СЕРИЯСЫ

♦

СЕРИЯ ХИМИИ И ТЕХНОЛОГИИ

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NAS RK is pleased to announce that News of NAS RK. Series of chemistry and technologies scientific journal has been accepted for indexing in the Emerging Sources Citation Index, a new edition of Web of Science. Content in this index is under consideration by Clarivate Analytics to be accepted in the Science Citation Index Expanded, the Social Sciences Citation Index, and the Arts & Humanities Citation Index. The quality and depth of content Web of Science offers to researchers, authors, publishers, and institutions sets it apart from other research databases. The inclusion of News of NAS RK. Series of chemistry and technologies in the Emerging Sources Citation Index demonstrates our dedication to providing the most relevant and influential content of chemical sciences to our community.

Қазақстан Республикасы Ұлттық ғылым академиясы "ҚР ҰҒА Хабарлары. Химия және технология сериясы" ғылыми журналының Web of Science-тің жаңаланған нұсқасы Emerging Sources Citation Index-те индекстелуге қабылданғанын хабарлайды. Бұл индекстелу барысында Clarivate Analytics компаниясы журналды одан әрі the Science Citation Index Expanded, the Social Sciences Citation Index және the Arts & Humanities Citation Index-ке қабылдау мәселесін қарастыруда. Webof Science зерттеушілер, авторлар, баспашылар мен мекемелерге контент тереңдігі мен сапасын ұсынады. ҚР ҰҒА Хабарлары. Химия және технология сериясы Emerging Sources Citation Index-ке енуі біздің қоғамдастық үшін ең өзекті және беделді химиялық ғылымдар бойынша контентке адалдығымызды білдіреді.

НАН РК сообщает, что научный журнал «Известия НАН РК. Серия химии и технологий» был принят для индексирования в Emerging Sources Citation Index, обновленной версии Web of Science. Содержание в этом индексировании находится в стадии рассмотрения компанией Clarivate Analytics для дальнейшего принятия журнала в the Science Citation Index Expanded, the Social Sciences Citation Index и the Arts & Humanities Citation Index. Web of Science предлагает качество и глубину контента для исследователей, авторов, издателей и учреждений. Включение Известия НАН РК в Emerging Sources Citation Index демонстрирует нашу приверженность к наиболее актуальному и влиятельному контенту по химическим наукам для нашего сообщества.

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A MODELING STUDY OF ALLENE OXIDATION AND PYROLYSIS

Abstract. The present work is an extension and upgrade of the earlier published detailed DLR reaction mechanism for the allene oxidation chemistry. Experimental data for ignition delay times obtained in shock tubes (ST), laminar flame speed data and species concentrations measured in laminar flames were used for the model revision and refinement. Threeoxygenated components C_3H_3OO, C_3H_2OOH, H_2CCHCO and their reactions, related to the lower temperature oxidation reactions, were newly included in the model. The thermodynamical properties of these species and reaction rate coefficients for $H_2CCCH+O_2 \leftrightarrows C_3H_3OO$, $C_3H_3OO \leftrightarrows C_3H_2OOH$ and $C_3H_2+HO_2 \leftrightarrows C_3H_2OOH$ were estimated using group additivity methods. The rate coefficients for most important reactions were revised on the basis of literature data; their uncertainty factors were estimated using statistical method. The developed mechanism was validated on the literature experimental data over parameters ranges of initial pressure 0.03-10 atm, the temperature 300-2500 K, the equivalence ratio 0.7-1.7 for allene and its mixtures, such as allene/propyne, allene/metane, allene/acetylene. The obtained model reflects well experimental data, but there is some inconsistency between experimental data for ignition delay times. However, the performed improvements in the C_3H_4 oxidation chemistry led to progress in simulation of concentration profiles of the polyaromatic hydrocarbon (PAH) precursors.

Keywords: reaction mechanism, allene, oxidation, ignition, flame.

Introduction

Better understanding of the C_3 hydrocarbon oxidation is an important scientific topic, due to two reasons: they are key intermediates in the combustion of hydrocarbon fuels such as propane, n-butane, n-heptane and iso-octane [1-3], and play an active role in the propargyl formation, which is one of the most important PAH precursors.

Allene is a significant intermediate in the combustion of propene. The resonantly stabilized propargyl (H_2CCCH) radical, which plays the major role in formation of first aromatic molecule, benzene (A1), is formed mostly in reactions of the allene decomposition and H-atom abstraction. The literature analysis showed that only several studies, numerical and experimental [2,4-8] were addressed to the C_3H_4 combustion.

Fournet et al. [5] measured the ignition delay times of allene and propyne behind reflected shock waves in the temperature range of 1000-1650 K and the rather narrow pressure range of 8.5-10 atm. On this basis, their reaction mechanism for acetylene, propyne, allene and 1,3-butadiene was developed [5]. Besides their measured data [5], experiments on the species concentration profiles obtained in premixed flames with fuels such as acetylene by Bastin et al. [9], Westmoreland et al.[10], and 1,3-butadiene by Cole et al. [11] premixed flames were used for the allene sub-mechanism [5]validation.

Faravelli et al. [7] studied the oxidation of propyne and allene in a jet-stirred reactor (JSR) and proposed the chemical kinetic scheme for the C_3H_4 oxidation at the intermediate- and high-temperature regions. Faravelli et al. [7]shown that the isomerization reactions proceeding via direct and H addition routes are significant in the oxidation. The developed reaction scheme has been tested on the experimental results obtained in ST experiments of Curran et al. [4], laminar flame of Miller et al. [12]and JSR [7].

Petrova et al. [8] proposed a detailed chemical-kinetic mechanism for the high-temperature combustion of allene. It was shown that the combustion properties of allene and propyne are quite similar and their ignition times measured in shock tubes are practically identical. The mechanism [8]was verified against ST experimental data [4] and laminar flame speed data of Davis et al. [6].

The most detailed study was recently published by Vourliotakis et al. [2]. They extensively studied existing uncertainties regarding the C_3H_4 isomers chemistry and tested their model on the ST ignition delay data [4]and on concentration species investigated by Hansen and co-workers [13,14] in laminar flamesof allene and propyne. It was concluded [2] that the dynamics of allene and propyne breakdown are more dependent on the initial stoichiometry, and less dependent on the isomeric structure.

The present study is a part of the on-going work aimed at optimizing the PAH kinetic mechanism formation [15-17] and reports results of the C_3H_4 sub-model upgrade at lower temperature, i.e. the second stage in the planned C_3 oxidation chemistry updating. The reaction model was improved on the experimental data for ignition delay times obtained in the shock tubes, laminar flame speed data and species concentrations measured in laminar flames. Overall integrated parameter ranges were: initial pressure 0.03-10 atm, the temperature 300-2500 K, the equivalence ratio 0.7-1.7 for allene and its mixtures, such as allene/methane, and allene/acetylene.

Kinetic Model

The detailed chemistry of C_3H_4 sub-model is a part of earlier published C_3H_4 sub-mechanism of Auyelkhankyzy et al. [15]at high-temperature, which consists of 111 species and 926 reversible elementary reactions including the PAH chemistry up to 5-ring molecules. The C_3H_4 sub-model upgrade was carried out through the model optimization based on the experimental data from [4-6,12,13,18]. The numerical calculations have been performed with Chemkin [19] and Chemical Workbench [20] software. Constant-volume, homogeneous, and adiabatic conditions behind the reflected shock wave have been used to model the shock tube experiments.

First simulations of ignition delay times revealed that the model [15] does not reproduce correctly ignition delay data for lower temperatures: in this case 1100-1350 K. It was found out that the oxidation of allene at lower temperature was inhibited with the H_2CCCH formation. This has been explained with a disbalance between the chain-branching reactions of a prompt dissociation and the chain propagation by bimolecular reactions of chemically activated species.

The chain propagation bimolecular reactions being in the model

$$H_2CCCH+O_2 \leftrightarrow CH_2CO + HCO \quad (R1)$$
$$H_2CCCH+O_2 \leftrightarrow CH_3CO + CO \quad (R2)$$
$$H_2CCCH+O_2 \leftrightarrow C_2H_3 + CO_2 \quad (R3)$$

are very important at high-temperature oxidation [18], but they did not influence the low-temperature oxidation. The reaction channels which could contribute to propargyl consumptions significantly have not found. According to the general reaction schemes [21,22]for low-temperature oxidation, we supposed to include the peroxy radical, C_3H_3OO, formation in the studied model

$$H_2CCCH+O_2 \leftrightarrows C_3H_3OO \quad (R4)$$

The following sequence converts peroxy radicals to other radicals

$$C_3H_3OO \leftrightarrows C_3H_2OOH \quad (R5)$$
$$C_3H_3OO \leftrightarrows H_2CCHCO+O \quad (R6)$$
$$C_3H_2+HO_2 \leftrightarrows C_3H_2OOH \quad (R7)$$

Four oxygenated components C_3H_3OO, C_3H_2OOH, H_2CCHCO, and C_3H_2O were finally included in the model. The presence of H_2CCHCO in the system has been shown in the study of Nguyen et al. [17], who investigated the H_2CCHCO radical formation by oxygen attack of C_3H_4.

The reaction rate coefficients for (R4), (R5) and (R7) have been evaluated applying group additivity methods [23].The rate coefficient of (R6) was evaluated by analogy with similar reaction,

$CH_2CHOO=CH_2CHO+O$, studied by Goldmith et al. [24] and finally the *k6* was multiplied to 10. The modification in the DLR mechanism [15] conducted in the present work is shown in Table 1.

Table 1 - Modifications in the DLR mechanism conducted in the present work

	Reaction	*k*, cm^3,s, mole, K			Ref.
		A	n	E_a	
R4	$H_2CCCH+O_2⇆C_3H_3OO$	6.000E+12	0.00	0.00	This work
R5	$C_3H_3OO⇆C_3H_2OOH$	2.032e+08	1.14	17395.0	This work
R6	$C_3H_3OO⇆H_2CCHCO+O$	5.220E+30	-4.71	21170.0	See text
R7	$C_3H_2+HO_2⇆C_3H_2OOH$	1.000e+13	0.00	0.00	This work
R8	$H_2CCCH+H_2O⇆CH2CHCHO+H$	6.000E+12	0.00	1042.0	[2]
R9	$CH_2CHCHO+H⇆H_2CCHCO+H_2$	1.150E+13	0.00	12107.3	[25]
R10	$CH_2CHCHO+OH⇆H_2CCHCO+H_2O$	8.000E+14	0.30	8304.0	[25]
R11	$H_2CCHCO⇆C_2H_3+CO$	1.000E+15	0.00	8304.0	[25]
R12	$H_2CCCH +O⇆C_3H_2O+H$	2.100E+14	0.00	17300.0	[2]
R13	$H_2CCCH +OH⇆C_3H_2O+H_2$	1.400E+14	0.00	0.00	[2]
R14	$C_3H_2O⇆C_2H_2+CO$	1.200E+13	0.00	0.00	[2]
R15	$C_3H_2O+O⇆HCO+HCCO$	8.510E+14	0.00	35722.9	[2]
R16	$C_3H_2O+OH⇆HCO+CH_2CO$	1.000E+13	0.00	0.00	[2]
R17	$H_2CCHCO+H⇆C_3H_2O+H_2$	1.000E+13	0.00	0.00	[2]
R18	$H_2CCHCO+O⇆C_3H_2O+OH$	6.000E+13	0.00	0.00	[2]

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

Results

Ignition of $C_3H_4/O_2/Ar$ mixtures

The simulations of experimental data [4,5] identified some discrepancies between these two data sets. Despite the similar initial temperature and identical mixture compositions, the results obtained in these studies demonstrate quite different trends. The data from [5], Fig.1, shows the faster ignition than it was observed in [4] for temperature >1650 K, and are slower than data [4] at temperature lower than 1350 K under similar conditions for equivalence ratio. The faster observations can be logically explained with the higher pressure. One possible explanation for the deaccelerating of the ignition delay time with the pressure growth could bean increasing the HO_2 production caused by higher pressure, i.e. p_5=8.5-10.0 atm, in experiment [5], in comparison to p_5=2.1, 3.5 and 5.0atm in experiment [4]. However, at studied temperatures [4,5], T_5 = 1350-1850K, this effect is no longer so strong to slowdown the ignition delay time with factor of 2.5, as it follows from the experimental data comparison, Fig.1.The sensitivity analysis has been carried out by changing the rate constant of $C_3H_4+HO_2⇆H_2CCCH+H_2O_2$ in ranges defined with uncertainty analysis [15]. The results of this analysis indicate the nonsignificant influence of this reaction in contribution to the changing of the ignition trends. This analysis can indicate on the possible inconsistency of these two datasets.

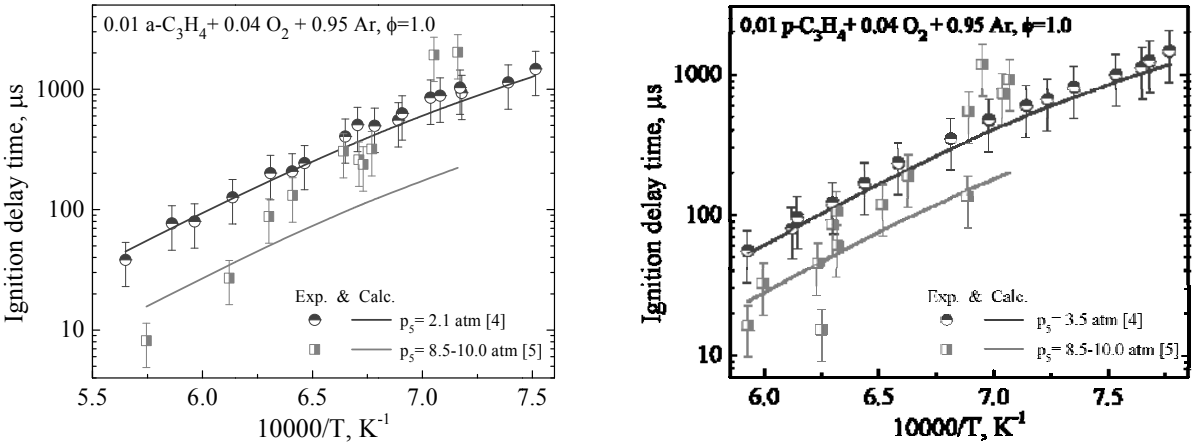

Figure1 - Comparison between computed and experimental [4,5] ignition delay times of $C_3H_4/O_2/Ar$

The introduced reactions (R4)-(R7) improved sufficiently the simulations of data from Curran et al. [4]for T_5<1350 K, Fig.1, and increased the disagreement with data of Fournet et al. [5]for these temperatures: the model under-predicts measurements from [5]. Calculated values, as it was described above, were used for k_4, k_5, k_7 without any changes. The rate constant k_6 was multiplied to 10 to accelerate the ignition simulations at lower temperatures.

The obtained progress in experimental data reproduction is shown in the Fig. 2. The least square residual for ignition delay time calculated with initial model and with the present one was reduced from 8.03E+01 to 2.96E+01.

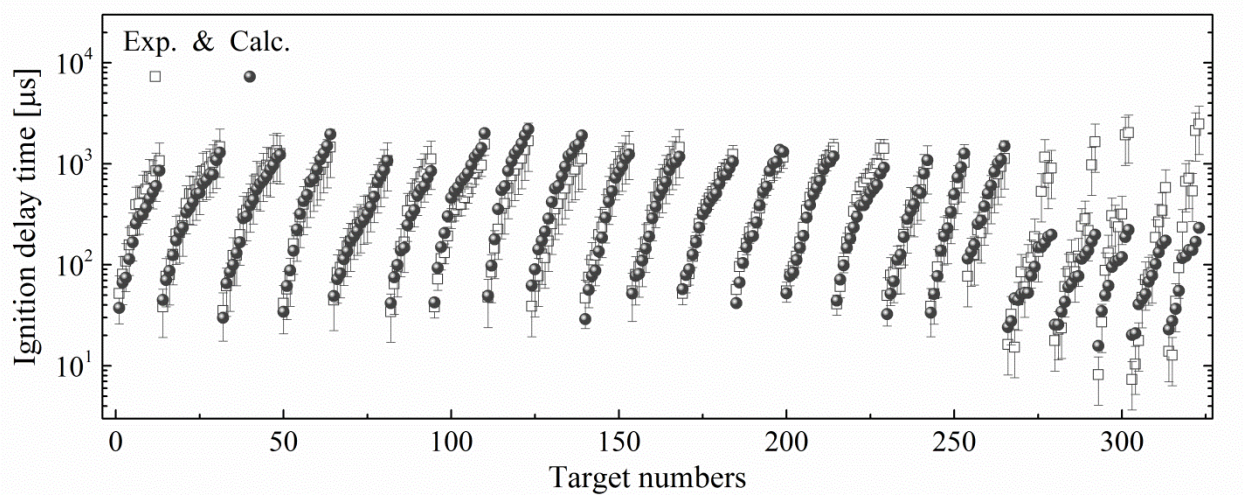

Figure 2 - Comparison between computed models and experimental ignition delay times of $C_3H_4/O_2/Ar$ [4,5]

Laminar flame speed of C_3H_4/air mixtures

The present mechanism validated on the basis of the experimental data by Davis et al. [6], which studied the oxidation of propyne/(18% O_2 in N_2) mixtures in laminar premixed flames using the counter-flow twin flame configuration. The sensitivity analysis is populated with reactions of hydrogen and C_1 hydrocarbon species, and there are only a few reactions of allene and propargyl that influence laminar flame speed at all stoichiometric conditions. The addition of the reactions (R4)-(R8) to the mechanism lead to nonsignificant change in the laminar flame speed data at lean to rich equivalence ratio. This modification leads to predict the shape of the laminar flame speed curve reasonably well. The results are shown in [15].

Concentration species of $C_3H_4/O_2/Ar$ mixtures

A successful reproduce the ignition delay times of both allene and propyne mixtures and laminar flame speed data for propyne leads to main goal of this study; it is to describe the major and intermediate species formed in flames and to improve the reaction pathways of PAH formation and growth in modelling tools to predict soot precursors formation in allene flame.

The initially validated against species concentration profiles data results show in excellent agreement for major stable species, such as C_3H_4, O_2, Ar, H_2, H_2O, CO, CO_2 in all flames. The model over-predicts the CH_3 and CH_4 mole fractions obtained from [13], but the experimental data observed from [12]accurately reproduced very well, Fig. 3. It can be explained, as it noted from [13], in experimental data obtained from [13]mole fractions of these components no detectable amount in the post-flame region.

Concentration profiles of C_2H_2, C_2H_3, C_2H_4, and C_2H_6 was obtained from [18] and [13]. Mole faction of C_2H_2 obtained from [13] predicted quite accurately, but experimental data obtained from [18] is over-predicted almost 2 times. The data between each other is not consistent. Lower mole faction for C_2H_3 is observed with the present model compare the experimental data [13]. The mole fraction profiles for C_2H_4 and C_2H_6 obtained in both experimental data from [13,18] model reproduced in excellent agreement. Figure 4 shows the comparing of the experimental data and modeling results of C_2H_2 and C_2H_4.

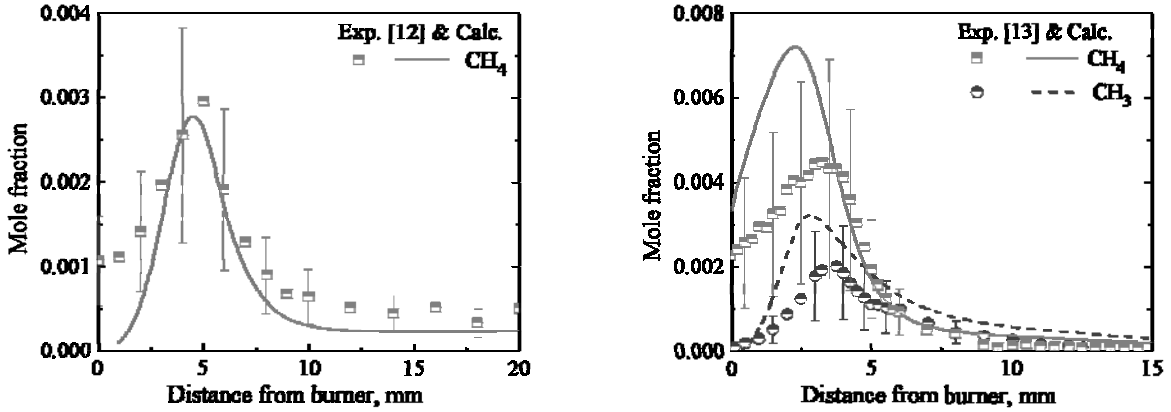

Figure 3 - Experimental (symbol) [12,13] and computed (line) mole fraction profiles of CH_3 and CH_4 in $C_3H_4/O_2/Ar$ flame

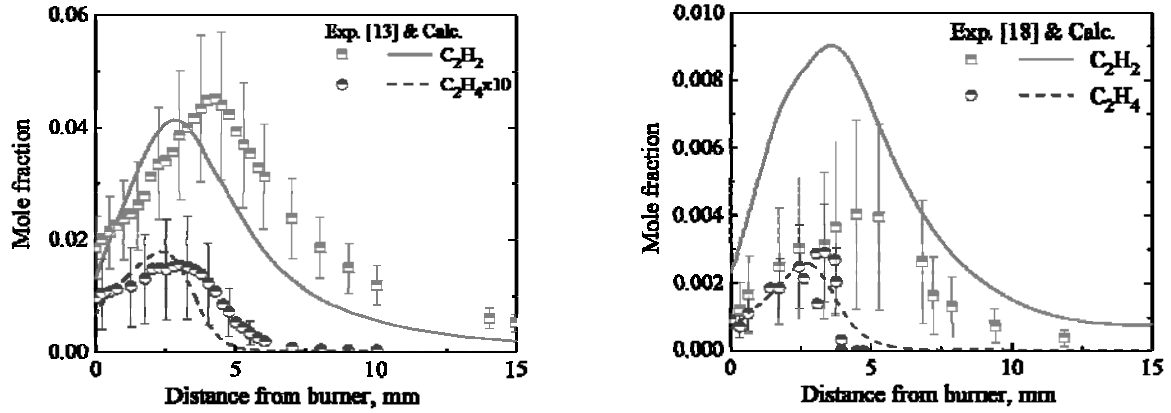

Figure 4 - Experimental (symbol) [13,18] and computed (line) mole fraction profiles of main and intermediate species in $C_3H_4/O_2/Ar$ flame

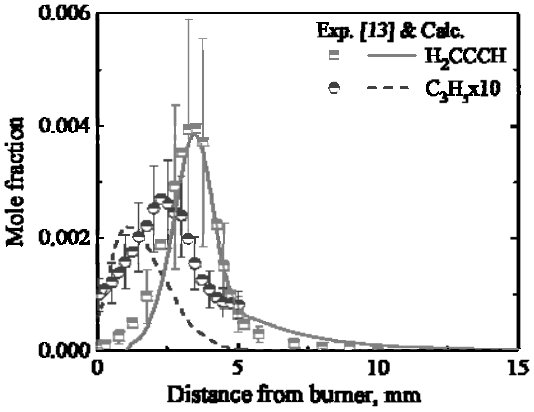

Figure 5 - Mole fraction profiles of H_2CCCH and C_3H_5 in $C_3H_4/O_2/Ar$ flame [13]

Nevertheless, the detection the isomeric composition for C_3 hydrocarbons [13] in allene flame we have only singlet propargylene (HCCCH) as C_3H_2 and allene as C_3H_4 in present model. The first reason is the objective of achieving simplifications and secondly is the indistinguishable behavior of the ignition of allene and propyne. Predicted and experimentally derived mole fractions profiles for radicals C_3H_3 and C_3H_5 are in excellent agreement, Fig. 5. The C_3H_2 mole fractions peak at experiment is $1.00x10^4$, but prediction is $2.25x10^4$. The present model is over-predicted the mole fraction profiles for molecules C_3H_6 and C_3H_8 obtained from [18]. It is the next goals.

The present model reproduced lower mole fractions profiles for C_4H_2 obtained [13] and [12], Fig.6. Mole fractions profiles for C_4H_4 obtained from [13] and [12] is inconsistency, for data obtained from [13] model is under-predicted, but for data from [18] model is over-predicted. Mole fraction profiles for C_4H_5 obtained from [13] are $2.00x10^4$, but prediction is 2 times high. C_4H_8 mole fractions profiles obtained from [18] predicted accurately. The C_5H_5 mole fractions peak at experiment is $1.50x10^4$ from [13] but prediction is $7.50x10^5$.

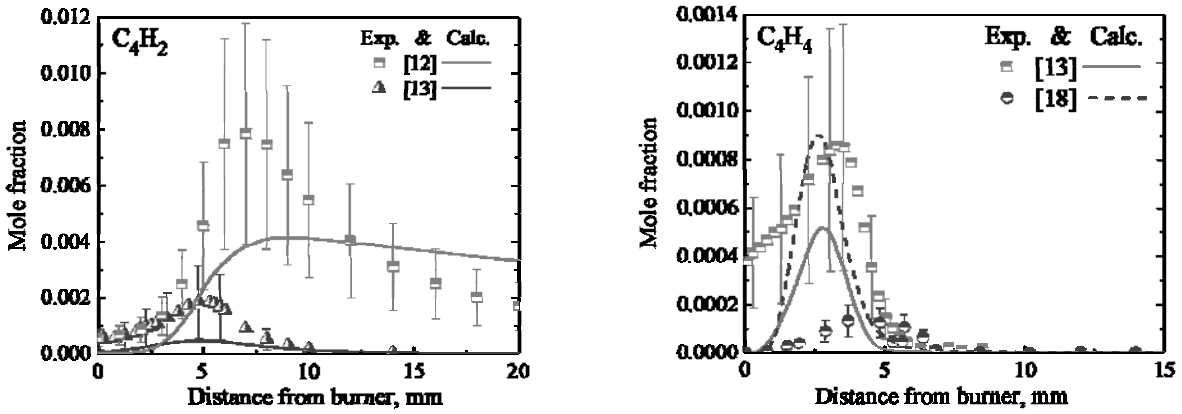

Figure 6 - Experimental (symbol) [12,13,18] and computed (line) mole fraction profiles of C_4H_2 and C_4H_4 in $C_3H_4/O_2/Ar$ flame

Prediction the concentration profiles of benzene is too high for all these three flames. The prediction of benzene profiles is possible after developing the sub-models to propene and propane.

Conclusions

A new detailed kinetic mechanism has been proposed to model the oxidation of allene and their mixtures. The mechanism for allene is derived from recent mechanisms for the oxidation of acetylene and allene and has been successfully validated using experimental results obtained in a shock tube reactor and in laminar flames. The mechanism for the mixture can qualitatively reproduce the evolution of the ignition delay times, laminar flame speed, and species concentration profiles observed. Three more of the missing reactions with propargyl radical, which is not been previously reported in the literature have been added. Addition of these reactions is given possibility reproduced the ignition delay time at lower temperatures. Unfortunately, due to non-availability the experimental data of the oxidation of allene at low-temperature T > 1000 K do not impossible to validate the mechanism. The hierarchical structure of present C_3H_4 sub-mechanism will be used for further developing a sub-mechanism for propene that is consistent with the available experimental combustion data for this fuel; then, finally, keeping these mechanisms fixed, find a successful mechanism for propane.

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АЛЛЕННІҢ ТОТЫҒУЫН ЖӘНЕ ПИРОЛИЗІН МОДЕЛЬДІК ЗЕРТТЕУ

Аннотация. Осы мақалада НАО-ның реакциялық механизмі негізінде алленнің тотығуының химиялық реакциялары кеңейтілді және жаңартылды. Реакциялық механизмді тексеру және оңтайландыру үшін соққы түтігінде алынған тұтану уақыты бойынша, ламинарлы жалын жылдамдығы бойынша және компоненттердің концентрацияларының профильдері бойынша алынған эксперименттік деректер қолданылды. Нәтижесінде, алленнің төмен температурада тотығуын сипаттау үшін механизмге жаңадан үш оттегімен байытылған C_3H_3OO, C_3H_2OOH, H_2CCHCO компоненттері және олардың реакциялары енгізілді. Осы компоненттердің

термодинамикалық қасиеттері және $H_2CCCH+O_2 \leftrightarrows C_3H_3OO$, $C_3H_3OO \leftrightarrows C_3H_2OOH$, $C_3H_2+HO_2 \leftrightarrows C_3H_2OOH$ реакцияларының жылдамдығының коэффициенттері топтық қосынды әдісі арқылы бағаланды. Ең маңызды реакциялардың жылдамдық коэффициенттері әдеби деректер негізінде қайта қаралды және олардың белгісіздік факторлары статистикалық өңдеу арқылы бағаланды. Өңделген модель әдеби тәжірибелік деректер негізінде қысым 0.03-10 атм, температура 300-2500 К және эквиваленттік қатынасы 0,7-1,7 тең аллен және олардың қоспалары аллен/пропин, аллен/метан және аллен/ацетилен негізінде тексерілді. Алынған модель эксперименттік деректерді жақсы сипаттайды, бірақ тұтану уақыттары бойынша эксперименттік деректер арасында сәйкессіздік бар. Алайда, C_3H_4 тотығуының химиялық реакцияларының кеңейтілуі полиароматты көмірсутектердің (ПАК) концентрацияларының профильдерін толық сипаттауға әкелді.

Тірек сөздер: реакциялық механизм, аллен, тотығу, тұтану, жалын

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МОДЕЛИРОВАНИЕ ОКИСЛЕНИЯ И ПИРОЛИЗА АЛЛЕНА

Аннотация. Настоящая работа посвящена расширению и улучшению ранее опубликованного подробного механизма реакции DLR для химии окисления аллена. Экспериментальные данные по временам задержек воспламенения полученных в ударных трубах, данные по скоростям ламинарных пламен и профилям концентрации компонентов, полученных в ламинарных пламенах, были использованы для тестирования и оптимизации реакционного механизма. Три оксигенированные компоненты C_3H_3OO, C_3H_2OOH, H_2CCHCO и их реакции, которые важны для низкотемпературного окисления, были впервые включены в настоящую модель. Термодинамические свойства этих компонентов и коэффициенты скорости реакции $H_2CCCH+O_2 \leftrightarrows C_3H_3OO$, $C_3H_3OO \leftrightarrows C_3H_2OOH$ и $C_3H_2+HO_2 \leftrightarrows C_3H_2OOH$ были оценены с использованием метода групповой аддитивности. Коэффициенты скорости для наиболее важных реакций были пересмотрены на основе литературных данных и их коэффициенты неопределенности оценивались с использованием статистического метода. Разработанный механизм был подтвержден литературными экспериментальными данными при давлении 0,03-10 атм, температуре 300-2500 К, и при коэффициенте эквивалентности 0,7-1,7 для аллена и его смесей, таких как аллен/пропин, аллен/метан, аллен/ацетилен. Полученная модель удовлетворительно воспроизводит экспериментальные данные, но есть некоторые несогласованность между экспериментальными данными по временам задержек воспламенения. Однако выполненные улучшения в химии окисления C_3H_4 привели к прогрессу в моделировании профилей концентрации полиароматических углеводородов (ПЦАУ).

Ключевые слова: реакционный механизм, аллен, окисление, воспламенение, пламя.

МАЗМҰНЫ

Ергожин Е.Е., Бектенов Н.Ә., СенГупта Аруп К., Байдуллаева А.Қ., Садыков Қ.А., Әбдралиева Г.Е., Қалмуратова К.М., Рыспаева С.Б. Эпоксиакрилат пен комплексондар негізіндегі жаңа комплекстүзгіш ион алмастырғыштар арқылы стронций иондарын сорбциялау (ағылшын тілінде)..... 6

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