
Article:
Messaoudani, Z.L., Hamid, M.D., Hassan, C.R.C. et al. (1 more author) (2020) The effects of hydrogen addition on the chemical kinetics of hydrogen-hydrocarbon flames : a computational study. South African Journal of Chemical Engineering, 33. pp. 1-28. ISSN 1026-9185

https://doi.org/10.1016/j.sajce.2020.03.003

South African Journal of Chemical Engineering 33 (2020) 1–28

Contents lists available at ScienceDirect

South African Journal of Chemical Engineering

journal homepage: www.elsevier.com/locate/sajce

The effects of hydrogen addition on the chemical kinetics of hydrogen-hydrocarbon flames: A computational study

Zine labidine Messaoudani[a,*], Mahar Diana Hamid[a,*], Che Rosmani Che Hassan[a], Yajue WU[b]

[a] Department of Chemical Engineering,Faculty of Engineering, University Malaya, Kuala lumpur 50603, Malaysia
[b] Department of Chemical and Biological Engineering, Sheffield University, United kingdom

ARTICLE INFO

Keywords:
Hydrogen
Hydrogen-hydrocarbon jet flames
Stability limits
Turbulent diffusion flames
Chemical kinetics

ABSTRACT

In this paper, the effects of hydrogen addition on the chemical kinetics of hydrogen–hydrocarbon flames were investigated numerically. Profiles of maximum OH, O and H radical mole fractions, flame temperature and emission levels of hydrogen-methane, hydrogen-ethane and hydrogen-propane flames were computational obtained using Kintecus solver code. The simulations were performed by incorporating Konnov's hydrocarbon combustion mechanism at the stoichiometric condition and the constant pressure of 1 atm. It was found that a small hydrogen increase in the flame mixture can modestly affects the temperature and mole fraction profiles, however, the significant increase can be observed upon 40%, 60% and 80% of hydrogen addition for hydrogen-methane, hydrogen-ethane and hydrogen-propane flames respectively can lead to decrement of CO and CO_2 emissions but increment in the combustion kinetics and the adiabatic flame temperature plus an extension of the flame stability limits. A comparison of the flames free radical profiles and the laminar burning velocity of the flames showed a strong correlation.

1. Introduction

In recent years, hydrogen started to play an important role in either as a fuel for fuel cell usage or as an additive to enhance the combustion performance of hydrocarbon fuels. Although hydrogen has been used in the aerospace and commercial industry for many years, there are many gaps still need to be overcome before allowing hydrogen usage by the public (Messaoudani, 2016). Hydrogen has been considered as a potential clean energy carrier, thus creating the term 'hydrogen economy'.

The wider flammability limit and lower volumetric density of hydrogen make it difficult to store and supply. At NTP, the volume of hydrogen gas needed to deliver the same amount of energy as methane is within a factor of 4. This issue can be solved by storing hydrogen either as CGH_2 in hydrogen tank at high pressure (700 to 900 bar) or as LH_2 in cryogenic hydrogen tank at a very low temperature of 20.28 K. However, this extreme storage and handling measures pose several safety issues and hazards to the public.

In order to use hydrogen as an energy carrier, we must ensure that it is safe enough and can be used in the existing combustion applications without creating any other high risks (Rigas and Amyotte, 2012, 2013). This can be achieved by the complete understanding of the combustion characteristics and the events that might occur in case of accidental releases of hydrogen into the atmosphere and/or mix with other gaseous fossil fuels in the surrounding environment (Messaoudani, 2016). Therefore, it is important to elucidate the effects of hydrogen addition to hydrocarbon fuels on its chemical kinetics and emission levels.

Laminar burning velocity is an important parameter in the flame study as it is strongly related to the flame combustion kinetics; fuel with a higher value of burning velocity indicates a faster overall chemical reaction. Due to its significant role in the combustion field, laminar burning velocities of various fuels have been experimentally determined extensively for the past 60 years. Pioneering work of Lewis and von Elbe (Von Elbe and Lewis, 1948) on the burning velocity of various hydrocarbons had subsequently enabled other researchers to further elaborate the parameter. There are four primary experimental methods used to determine flame burning velocity; (1) the Bunsen burner method, (2) the constant volume spherical bomb method, (3) the soap bubble method, and (4) the flat flame burner method. However, due to several discrepancy issues such as tube wall quenching and heat loss from electrodes, the Bunsen burner and the soap bubble method are less favourable compare other two methods. The majority of researchers have employed the constant volume spherical bomb method (Stone et al., 1998, Daly et al., 2001, Ilbas et al., 2006, Liao et al., 2007, Bradley et al., 2007, Reyes et al., 2018, Hinton et al., 2018, Faghih and Chen, 2016, Lamoureux et al., 2003, Nair and Gupta, 1974, Lipatnikov et al., 2015, Reyes and Tinaut, 2017) and the flat flame method (Yumlu, 1967, Sher and Ozdor, 1992, El-Sherif, 1998,

* Corresponding authors.
E-mail addresses: m.zinou2015@gmail.com (Z.l. Messaoudani), mahar.diana@um.edu.my (M.D. Hamid).

https://doi.org/10.1016/j.sajce.2020.03.003
Received 22 January 2020; Received in revised form 5 March 2020; Accepted 25 March 2020

Nomenclature

Abbreviation Description

A	The frequency factor
CH_4	Methane
CGH_2	Compressed hydrogen in gaseous state
C_2H_6	Ethane
C_3H_8	Propane
E_a	Activation energy
H_2	Hydrogen
H_2O	Water
HO_2	Hydroperoxyl
H_2O_2	Hydrogen peroxide
K	The coefficient rate
LH_2	Liquid hydrogen
NTP	Normal Temperature and Pressure (20 °C and 101.3 kPa)
NOx	Nitrogen oxides
O	Oxygen
OH	Hydroxide
R	Gas constant
T	Temperature

Turkeli-Ramadan et al., 2017, Günther and Janisch, 1972, Gillespie et al., 2012) to obtain the laminar burning velocity of various fuel mixtures.

Generally, the values of laminar burning velocities for each of the pure hydrocarbon and hydrogen flames are quite abundant but it is notably difficult to obtain the laminar burning velocities for hydrocarbon-hydrogen flames. Therefore, in this study, it is convenient to compile the laminar burning velocity according to the flames and primary fuels. A compilation of various experimentally obtained laminar burning velocities for H_2-CH_4, H_2-C_2H_6 and H_2-C_3H_8 flames at equivalence ratio equals to one has been conducted and will be further elaborated in the following sections.

In the past decades,the kinetic mechanisms of hydrogen flames have been investigated extensively (Pang and Li, 2016, Luo and Liu, 2017, Liu, 2014, Zhou et al., 2016, Korsakova et al., 2016, Luo and Liu, 2016, de Ferrières et al., 2013). It has been well established and involves eight reacting species (H_2, O_2, H, O, OH, HO_2, H_2O_2 and H_2O). The kinetic mechanisms of hydrocarbon combustion are complicated compared to hydrogen flames and it is expected to be even more complicated if the hydrogen is mixed with hydrocarbon fuel.

Several researchers (Hu et al., 2009, Fairweather et al., 2009, Wang et al., 2009, Hu et al., 2009) has studied the effects of hydrogen addition on the chemical kinetics of hydrogen-methane flames experimentally and relate it to the burning velocity of the flame. Particularly, Hu et al. (Hu et al., 2009) has stated that the enhancement of overall chemical reaction with the increase of hydrogen composition is closely related to the increase of free radical concentrations in the reaction zone. So far there is limited information about the kinetic of hydrogen-ethane and hydrogen-propane flames. According to Glassman (Glassman, 2008), in order to describe the chemical kinetics of hydrocarbon combustion at elevated temperature, several key factors, such as reactants decomposition reactions, radical reactions with reactants, chain branching reactions and recombination reactions, should be taken into consideration. In the study of the chemical kinetics of combustion process, information about the destruction and production of radicals of OH, O and H is very important because it shows the chemical kinetics of the fuels. The elementary kinetics involving chemical radicals, such as O, OH, H and HO_2, influence the trend of intermediate radical pool in a reacting system, which in turn, determines the physical combustion characteristics of a flame. Most previous study on chemical kinetics of hydrogen-hydrocarbon flames emphasized more on the OH radical (El-Sherif, 1998, Choudhuri and Gollahalli, 2004). However, these data are still not enough and further studies are needed to incorporate the changes that may happen to the chemical kinetics of fuel mixture due to the hydrogen addition.

The flame propagation speed in laminar flow is governed by chemical processes in which diffusion plays an important part. During the past 50 years, the need for better understanding of one-dimensional flame problems has been the stimulus to the refinement of kinetic mechanisms for combustion of both hydrogen and hydrocarbon mixtures. Detailed chemical kinetic mechanisms are employed to explain the conversion of reactants into products at the molecular level.

The work by Warnatz (Warnatz, 1985) compiled the combustion mechanism of propagating flames in alkane/alkene-air mixtures under lean and moderately rich conditions. This mechanism comes to 93 reactions which consist of the oxidation of hydrogen and monoxide carbon, the oxidation of C_1/C_2 hydrocarbons, and the oxidation of C_3 hydrocarbons. However, Hughes et al. (Hughes et al., 2001) have suggested that Warnatz mechanism is outdated and they had published a mechanism which is known as the Leeds mechanism that describes the oxidation kinetics of hydrogen, carbon monoxide, methane, ethane and ethene in flames and homogeneous ignition systems which consists of 351 irreversible reactions of 37 chemical species. Konnov (Konnov, 2000) had published a detailed reaction mechanism for methane and natural gas combustion which also deals with C_2 and C_3 hydrocarbons and their derivatives, N–H–O chemistry and NOx formation in flames. Another well-known hydrocarbon detailed kinetic mechanism is the GRI MECH which was developed by the team from University of California, Stanford University, the University of Texas, and SRI International (Smith et al., 2000). However, all these combustion mechanisms, except for Konnov's, do not include the N–H–O chemistry and NOx formation mechanism and would be less favourable in the case where we need to evaluate the NOx emission of the flames. Due to the argument presented, the author has chosen to use the Konnov's combustion mechanism in this study to simulate hydrogen-hydrocarbon combustion. The mechanism is presented in Table 1 in Appendix 1. The rate coefficient k can be expressed in the Arrhenius form as presented in Eq. 1:

$$k = AT^n \exp\left(-\frac{E_a}{RT}\right) \tag{1}$$

The values of A, n and E are included in Table A.1 for a specific reaction.

In this study, the chemical kinetics modelling of hydrogen-hydrocarbon combustion reactions was performed using the Kintecus solver code written by Dr. James Ianni. The code is relatively new compared to other chemical kinetics modelling software as it was only available by the early 2000s. Despite this, Kintecus has been used by many researchers to simulate combustion, nuclear, biological, enzyme, atmospheric and many other chemical kinetic and equilibrium processes. In addition, most of the early works conducted using Kintecus were mainly in the field of combustion kinetics (Hannebauer and Menzel, 2003, Park et al., 2004, Shafir et al., 2003). More recently, Huang and coworkers [in press43] have modelled the production of OH in propyl and oxygen combustion reaction using Kintecus and the results had shown good agreement with those obtained experimentally.

The previously mentioned issues are addressed by studying the changes that may occur on the chemical kinetics of hydrocarbon fuels due to the hydrogen addition. CH_4, C_2H_6 and C_3H_8 are used in this study due to its gaseous form at standard temperature and pressure, which enable it to be mixed readily with hydrogen prior to burning.

2. Computational methods

Kintecus solver code (Ianni and Bathe, 2003) was employed to model the reaction kinetics of the hydrogen-hydrocarbon flames. The detailed combustion mechanism of the hydrogen-hydrocarbon flames

Table. 1
Konnov's detailed hydrocarbon oxidation up to C_3.

No.	Reaction	A	Ea (cal/mol)	N
1	$H_2+M\leftrightarrow H+H+M$	6.50E+17	0	−1
2	$H+H+H_2\leftrightarrow H_2+H_2$	1.00E+17	0	−0.6
3	$O_2+M\leftrightarrow O+O+M$	1.00E+17	0	−1
4	$O+H+M\leftrightarrow OH+M$	6.20E+16	0	−0.6
5	$H_2+O_2\leftrightarrow OH+OH$	1.70E+13	48150	0
6	$O+H_2\leftrightarrow OH+H$	5.06E+04	6285	2.67
7	$H+O_2\leftrightarrow OH+O$	1.00E+14	14843	0
8	$H+O_2+M\leftrightarrow HO_2+M$	1.40E+18	0	−0.8
9	$H+OH+M\leftrightarrow H_2O+M$	2.20E+22	0	−2
10	$H_2+OH\leftrightarrow H_2O+H$	1.00E+08	3300	1.6
11	$OH+OH\leftrightarrow H_2O+O$	1.50E+09	100	1.14
12	$HO_2+OH\leftrightarrow H_2O+O_2$	1.90E+16	0	−1
13	$HO_2+O\leftrightarrow OH+O_2$	3.25E+13	0	0
14	$H+HO_2\leftrightarrow H_2+O_2$	4.22E+13	1411	0
15	$H+HO_2\leftrightarrow OH+OH$	1.70E+14	875	0
16	$H+HO_2\leftrightarrow H_2O+O$	3.00E+13	1700	0
17	$HO_2+HO_2\leftrightarrow H_2O_2+O_2$	4.20E+14	12000	0
18	$HO_2+HO_2\leftrightarrow H_2O_2+O_2$	1.30E+11	−1640	0
19	$OH+OH+M\leftrightarrow H_2O_2$	7.20E+13	0	−0.37
20	$H_2O_2+OH\leftrightarrow HO_2+H_2O$	1.70E+12	1320	0
21	$H_2O_2+H\leftrightarrow HO_2+H_2$	1.00E+13	3750	0
22	$H_2O_2+H\leftrightarrow H_2O+OH$	6.60E+11	3575	0
23	$H_2O_2+O\leftrightarrow HO_2+OH$	1.80E+14	4000	0
24	$N_2+O\leftrightarrow NO+N$	9.00E+09	76100	0
25	$N+O_2\leftrightarrow NO+O$	9.64E+14	6500	1
26	$NO+M\leftrightarrow N+O+M$	3.00E+11	148300	0
27	$NO+NO\leftrightarrow N_2+O_2$	1.26E+12	65000	0
28	$N_2O+M\leftrightarrow N_2+O$	1.00E+14	62620	0
29	$N_2O+O\leftrightarrow N_2+O_2$	6.92E+13	28200	0
30	$N_2O+O\leftrightarrow NO+NO$	1.00E+13	26630	0
31	$N_2O+N\leftrightarrow N_2+NO$	2.75E+14	20000	0
32	$N_2O+NO\leftrightarrow N_2+NO_2$	1.30E+15	50000	0
33	$NO+O+M\leftrightarrow NO_2$	3.91E+12	0	−0.75
34	$NO_2+O\leftrightarrow NO+O_2$	8.40E+11	−238	0
35	$NO_2+N\leftrightarrow N_2O+O$	1.00E+12	0	0
36	$NO_2+N\leftrightarrow NO+NO$	1.00E+12	0	0
37	$NO_2+NO\leftrightarrow N_2O+O_2$	3.95E+12	60000	0
38	$NO_2+NO_2\leftrightarrow NO+NO+O_2$	1.13E+04	27590	0
39	$NO_2+NO_2\leftrightarrow NO_3+NO$	1.33E+13	22720	2.58
40	$NO_2+O+M\leftrightarrow NO_3$	2.50E+06	0	0
41	$NO_3\leftrightarrow NO+O_2$	1.20E+11	12120	0
42	$NO_3+NO_2\leftrightarrow NO+NO_2+O_2$	1.02E+13	3200	0
43	$NO_3+O\leftrightarrow NO_2+O_2$	5.12E+11	0	0
44	$NO_3+NO_3\leftrightarrow NO_2+NO_2+O_2$	4.05E+18	4870	0
45	$N_2O_4+M\leftrightarrow NO_2+NO_2$	1.21E+12	12840	−1.1
46	$N_2O_4+O\leftrightarrow N_2O_3+O_2$	1.60E+09	0	0
47	$NO_2+NO+M\leftrightarrow N_2O_3$	2.71E+11	0	−1.4
48	$N_2O_3+O\leftrightarrow NO_2+NO_2$	3.70E+21	0	0
49	$N_2+M\leftrightarrow N+N+M$	2.65E+14	225000	−1.6
50	$NH+M\leftrightarrow N+H+M$	3.20E+13	75500	0
51	$NH+H\leftrightarrow N+H_2$	6.30E+11	325	0
52	$NH+N\leftrightarrow N_2+H$	2.54E+13	0	0.5
53	$NH+NH\leftrightarrow N_2+H+H$	8.00E+11	0	0
54	$NH+NH\leftrightarrow NNH+H$	2.00E+11	1000	0.5
55	$NH+NH\leftrightarrow NH_2+N$	1.00E+08	2000	0.5
56	$NH+NH\leftrightarrow N_2+H_2$	3.16E+23	0	1
57	$NH_2+M\leftrightarrow NH+H+M$	1.00E+14	91400	−2
58	$NH+H_2\leftrightarrow NH_2+H$	6.90E+13	20070	0
59	$NH_2+N\leftrightarrow N_2+H+H$	1.50E+15	0	0
60	$NH_2+NH\leftrightarrow N_2H_2+H$	1.00E+13	0	−0.5
61	$NH_2+NH\leftrightarrow NH_3+N$	5.00E+12	2000	0
62	$NH_2+NH_2\leftrightarrow NH_3+NH$	4.00E+13	10000	0
63	$NH_2+NH_2\leftrightarrow N_2H_2+H_2$	1.58E+12	12000	0
64	$N_2H_3+H\leftrightarrow NH_2+NH_2$	2.20E+16	0	0
65	$NH_3+M\leftrightarrow NH_2+H+M$	6.30E+14	93470	0
66	$NH_3+M\leftrightarrow NH+H_2+M$	5.42E+05	93390	0
67	$NH_3+H\leftrightarrow NH_2+H_2$	1.00E+11	9920	2.4
68	$NH_3+NH_2\leftrightarrow N_2H_3+H_2$	3.00E+08	21600	0.5
69	$NNH\leftrightarrow N_2+H$	1.00E+13	0	0
70	$NNH+M\leftrightarrow N_2+H+M$	4.00E+13	3060	0.5
71	$NNH+H\leftrightarrow N_2+H_2$	3.00E+13	3000	0
72	$NNH+N\leftrightarrow NH+N_2$	2.00E+11	2000	0
73	$NNH+NH\leftrightarrow N_2+NH_2$	1.00E+13	2000	0.5
74	$NNH+NH_2\leftrightarrow N_2+NH_3$	1.00E+13	0	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
75	$NNH + NNH \leftrightarrow N_2H_2 + N_2$	5.00E+16	10000	0
76	$N_2H_2 + M \leftrightarrow NNH + H + M$	3.16E+16	50000	0
77	$N_2H_2 + M \leftrightarrow NH + NH + M$	5.00E+13	99400	0
78	$N_2H_2 + H \leftrightarrow NNH + H_2$	1.00E+13	1000	0
79	$N_2H_2 + NH \leftrightarrow NNH + NH_2$	1.00E+13	1000	0
80	$N_2H_2 + NH_2 \leftrightarrow NH3 + NNH$	1.00E+11	4000	0
81	$N_2H_2 + NH_2 \leftrightarrow NH + N_2H_3$	1.00E+13	33780	0.5
82	$N_2H_2 + N2H2 \leftrightarrow NNH + N_2H_3$	1.00E+16	12000	0
83	$N_2H_3 + M \leftrightarrow NH_2 + NH + M$	1.00E+16	70000	0
84	$N_2H_3 + M \leftrightarrow N_2H_2 + H + M$	1.00E+12	49700	0
85	$N_2H_3 + H \leftrightarrow N_2H_2 + H_2$	1.00E+11	2000	0
86	$N_2H_3 + H \leftrightarrow NH + NH_3$	1.00E+11	0	0
87	$N_2H_3 + NH_2 \leftrightarrow NH_3 + N_2H_2$	1.00E+13	0	0.5
88	$N_2H_3 + N_2H_2 \leftrightarrow N_2H_4 + NNH$	1.00E+12	10000	0
89	$N_2H_3 + N2H3 \leftrightarrow NH_3 + NH_3 + N_2$	7.90E+13	0	0
90	$N_2H_4 + M \leftrightarrow NH_2 + NH_2$	1.00E+15	55000	0
91	$N_2H_4 + M \leftrightarrow N_2H_3 + H + M$	5.94E+12	80000	0
92	$N_2H_4 + H \leftrightarrow N_2H_3 + H_2$	4.46E+09	2380	0
93	$N_2H_4 + H \leftrightarrow NH_2 + NH_3$	6.15E+13	3100	0
94	$N_2H_4 + N \leftrightarrow N_2H_3 + NH$	1.00E+12	4000	0
95	$N_2H_4 + NH \leftrightarrow NH_2 + N_2H_3$	4.00E+10	2000	0.5
96	$N_2H_4 + NH2 \leftrightarrow N_2H_3 + NH_3$	2.50E+10	2000	0.5
97	$N_2H_4 + N2H2 \leftrightarrow N_2H_3 + N_2H_3$	2.80E+13	30000	0.5
98	$N + OH \leftrightarrow NO + H$	2.20E+14	0	0
99	$N_2O + H \leftrightarrow N_2 + OH$	6.70E+22	16750	0
100	$N_2O + H \leftrightarrow NH + NO$	5.50E+18	37155	−2.16
101	$N_2O + H \leftrightarrow NNH + O$	1.00E+12	47300	−1.06
102	$N_2O + OH \leftrightarrow N_2 + HO_2$	8.50E+12	17000	0
103	$HNO + NO \leftrightarrow N_2O + OH$	1.32E+14	29580	0
104	$NO_2 + H \leftrightarrow NO + OH$	1.81E+13	362	0
105	$NO_2 + OH \leftrightarrow HO_2 + NO$	4.64E+11	6676	0
106	$NO_2 + HO_2 \leftrightarrow HONO + O_2$	3.21E+12	−479	0
107	$NO_2 + H_2 \leftrightarrow HONO + H$	1.00E+13	28810	0
108	$NO_2 + NH \leftrightarrow N_2O + OH$	6.62E+13	0	0
109	$NO_3 + H \leftrightarrow NO_2 + OH$	1.39E+13	0	0
110	$NO_3 + OH \leftrightarrow NO_2 + HO_2$	5.55E+11	0	0
111	$NO_3 + HO2 \leftrightarrow HNO_3 + O_2$	1.51E+12	0	0
112	$NO_3 + HO2 \leftrightarrow NO_2 + OH + O_2$	2.52E+14	0	0
113	$N_2O_4 + H2O \leftrightarrow HONO + HNO_3$	3.79E+13	11590	0
114	$N_2O_3 + H2O \leftrightarrow HONO + HONO$	1.52E+15	8880	0
115	$H + NO + M \leftrightarrow HNO$	4.46E+11	0	−0.41
116	$HNO + H \leftrightarrow NO + H_2$	1.30E+07	655	0.72
117	$HNO + OH \leftrightarrow NO + H2O$	5.00E+11	−956	1.88
118	$HNO + O \leftrightarrow OH + NO$	5.00E+10	2000	0.5
119	$HNO + O \leftrightarrow NO_2 + H$	2.20E+10	2000	0
120	$HNO + O_2 \leftrightarrow NO + HO_2$	1.00E+11	9140	0
121	$HNO + N \leftrightarrow NO + NH$	5.00E+10	2000	0.5
122	$HNO + N \leftrightarrow H + N_2O$	5.00E+11	3000	0.5
123	$HNO + NH \leftrightarrow NH_2 + NO$	2.00E+13	0	0.5
124	$HNO + NH_2 \leftrightarrow NH_3 + NO$	3.63E-02	1000	0
125	$HNO + HNO \leftrightarrow N_2O + H_2O$	6.02E+11	1190	3.98
126	$HNO + NO_2 \leftrightarrow HONO + NO$	2.00E+12	2000	0
127	$NO + OH + M \leftrightarrow HONO$	1.40E+18	−721	−0.05
128	$NO_2 + H + M \leftrightarrow HONO + M$	1.20E+13	900	−1.5
129	$HONO + O \leftrightarrow OH + NO_2$	1.26E+10	5960	0
130	$HONO + OH \leftrightarrow H_2O + NO_2$	2.30E+12	135	1
131	$HONO + HONO \leftrightarrow H_2O + NO_2 + NO$	5.00E+12	8350	0
132	$HONO + NH_2 \leftrightarrow NO_2 + NH_3$	2.41E+13	0	0
133	$NO_2 + OH + M \leftrightarrow HNO_3$	2.23E+12	0	0
134	$NO + HO_2 + M \leftrightarrow HNO_3 + M$	1.03E+10	2200	−3.5
135	$HNO_3 + OH \leftrightarrow NO_3 + H_2O$	1.10E+06	−1240	0
136	$NH_3 + O \leftrightarrow NH_2 + OH$	5.00E+07	5210	2.1
137	$NH_3 + OH \leftrightarrow NH_2 + H_2O$	3.00E+11	950	1.6
138	$NH_3 + HO_2 \leftrightarrow NH_2 + H_2O_2$	8.00E+12	22000	0
139	$NH_2 + HO_2 \leftrightarrow NH_3 + O_2$	5.00E+12	0	0
140	$NH_2 + O \leftrightarrow H_2 + NO$	4.50E+13	0	0
141	$NH_2 + O \leftrightarrow HNO + H$	7.00E+12	0	0
142	$NH_2 + O \leftrightarrow NH + OH$	9.00E+07	0	0
143	$NH_2 + OH \leftrightarrow NH + H_2O$	8.00E+12	−460	1.5
144	$NH_2 + HO_2 \leftrightarrow HNO + H_2O$	4.50E+12	0	0
145	$NH_2 + O_2 \leftrightarrow HNO + OH$	9.30E+11	25000	0
146	$NH_2 + NO \leftrightarrow NNH + OH$	2.00E+20	0	0
147	$NH_2 + NO \leftrightarrow N_2 + H_2O$	3.20E+18	920	−2.6
148	$NH_2 + NO_2 \leftrightarrow N_2O + H_2O$	4.50E+13	0	−2.2
149	$NH + O \leftrightarrow NO + H$	4.50E+13	0	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
150	$NH + O \leftrightarrow N + OH$	2.00E+13	0	0
151	$NH + OH \leftrightarrow HNO + H$	5.00E+11	0	0
152	$NH + OH \leftrightarrow N + H_2O$	2.00E+13	2000	0.5
153	$NH + OH \leftrightarrow NO + H_2$	1.00E+13	0	0
154	$NH + HO_2 \leftrightarrow HNO + OH$	4.00E+13	2000	0
155	$NH + O_2 \leftrightarrow HNO + O$	7.80E+10	18000	0
156	$NH + O_2 \leftrightarrow NO + OH$	2.00E+13	1530	0
157	$NH + H_2O \leftrightarrow HNO + H_2$	2.00E+12	13850	0
158	$NH + N_2O \leftrightarrow N_2 + HNO$	5.60E+12	6000	0
159	$NH + NO \leftrightarrow NNH + O$	6.10E+13	10870	0.21
160	$NH + NO \leftrightarrow N_2 + OH$	1.00E+11	120	−0.5
161	$NH + NO_2 \leftrightarrow NO + HNO$	8.50E+13	4000	0.5
162	$N_2H_4 + O \leftrightarrow N_2H_2 + H_2O$	3.00E+10	1200	0
163	$N_2H_4 + OH \leftrightarrow N_2H_3 + H_2O$	2.00E+13	1290	0.68
164	$N_2H_3 + O \leftrightarrow N_2H_2 + OH$	3.00E+10	1000	0
165	$N_2H_3 + OH \leftrightarrow N_2H_2 + H_2O$	3.00E+12	1290	0.68
166	$N_2H_3 + O2 \leftrightarrow N_2H_2 + HO_2$	8.00E+12	0	0
167	$N_2H_3 + HO_2 \leftrightarrow N_2H_4 + O_2$	1.00E+13	0	0
168	$N_2H_2 + O \leftrightarrow NH_2 + NO$	2.00E+13	0	0
169	$N_2H_2 + O \leftrightarrow NNH + OH$	1.00E+13	1000	0
170	$N_2H_2 + OH \leftrightarrow NNH + H_2O$	3.00E+13	1000	0
171	$N_2H_2 + NO \leftrightarrow N_2O + NH_2$	1.70E+16	0	0
172	$NNH + O \leftrightarrow N_2 + OH$	2.40E+22	500	−1.23
173	$NNH + OH \leftrightarrow N_2 + H_2O$	1.20E+12	2444	−2.88
174	$NNH + O_2 \leftrightarrow N_2 + HO_2$	2.90E+11	150	−0.34
175	$NNH + O_2 \leftrightarrow N_2O + OH$	5.00E+13	150	−0.34
176	$NNH + NO \leftrightarrow N_2 + HNO$	1.50E+14	0	0
177	$CO + HO_2 \leftrightarrow CO_2 + OH$	1.17E+07	23650	0
178	$CO + OH \leftrightarrow CO_2 + H$	6.16E+14	−725	1.354
179	$CO + O + M \leftrightarrow CO_2 + M$	2.50E+12	3000	0
180	$CO + O_2 \leftrightarrow CO_2 + O$	1.56E+14	47800	0
181	$HCO + M \leftrightarrow H + CO + M$	1.00E+14	15760	0
182	$HCO + OH \leftrightarrow CO + H_2O$	3.00E+13	0	0
183	$HCO + O \leftrightarrow CO + OH$	3.00E+13	0	0
184	$HCO + O \leftrightarrow CO_2 + H$	9.00E+13	0	0
185	$HCO + H \leftrightarrow CO + H_2$	1.20E+10	0	0
186	$HCO + O_2 \leftrightarrow CO + HO_2$	1.20E+14	1190	0
187	$HCO + CH_3 \leftrightarrow CO + CH_4$	3.00E+13	0	0
188	$HCO + HO_2 \leftrightarrow CO_2 + OH + H$	3.00E+13	0	0
189	$HCO + HCO \leftrightarrow CH_2O + CO$	3.00E+12	0	0
190	$HCO + HCO \leftrightarrow H_2 + CO + CO$	2.40E+16	0	0
191	$CH_4 + M \leftrightarrow CH_3 + H$	2.40E+16	104913	0
192	$CH_4 + M \leftrightarrow CH_3 + H$	9.00E+12	104913	0
193	$CH_4 + HO_2 \leftrightarrow CH_3 + H_2O_2$	1.55E+07	24641	0
194	$CH_4 + OH \leftrightarrow CH_3 + H_2O$	7.20E+08	2774	1.83
195	$CH_4 + O \leftrightarrow CH_3 + OH$	1.30E+04	8485	1.56
196	$CH_4 + H \leftrightarrow CH_3 + H_2$	4.30E+12	8050	3
197	$CH_4 + CH_2 \leftrightarrow CH_3 + CH_3$	4.00E+13	10038	0
198	$CH_4 + O_2 \leftrightarrow CH_3 + HO_2$	1.00E+16	56900	0
199	$CH_3 + M \leftrightarrow CH_2 + H + M$	1.00E+16	90600	0
200	$CH_3 + M \leftrightarrow CH + H_2 + M$	8.00E+12	85240	0
201	$CH_3 + HO_2 \leftrightarrow CH_3O + OH$	2.64E+19	0	0
202	$CH_3 + OH \leftrightarrow CH_2OH + H$	5.74E+12	8068	−1.8
203	$CH_3 + OH \leftrightarrow CH_3O + H$	8.90E+18	13931	−0.23
204	$CH_3 + OH \leftrightarrow CH_2 + H_2O$	3.19E+12	8067	−1.8
205	$CH_3 + OH \leftrightarrow CH_2O + H_2$	8.43E+13	10810	−0.53
206	$CH_3 + O \leftrightarrow H + CH_2O$	3.40E+11	0	0
207	$CH_3 + O_2 \leftrightarrow CH_2O + OH$	1.32E+14	8940	0
208	$CH_3 + O_2 \leftrightarrow CH_3O + O$	3.80E-07	31400	0
209	$CH_3 + CH_3 + M \leftrightarrow C_2H_5 + H$	9.21E+16	7710	4.838
210	$CH_3 + CH_3 + M \leftrightarrow C_2H_6$	2.41E+13	636	−1.174
211	$CH_3 + CH_3O \leftrightarrow CH_4 + CH_2O$	2.41E+12	0	0
212	$CH_3 + CH_2OH \leftrightarrow CH_4 + CH_2O$	6.00E+13	0	0
213	$CH_3 + H \leftrightarrow SCH_2 + H_2$	7.80E+08	15100	0
214	$CH_3 + O_2 + M \leftrightarrow CH_3O_2$	1.00E+14	0	1.2
215	$CH_3 + CH_3 \leftrightarrow C_2H_4 + H_2$	7.20E+12	32000	0
216	$CH_3 + OH \leftrightarrow SCH_2 + H_2O$	2.50E+13	2780	0
217	$CH_2 + OH \leftrightarrow CH_2O + H$	4.80E+13	0	0
218	$CH_2 + O \leftrightarrow CO + H_2$	7.20E+13	0	0
219	$CH_2 + O \leftrightarrow CO + H + H$	5.00E+13	0	0
220	$CH_2 + O \leftrightarrow CH + OH$	8.00E+13	0	0
221	$CH_2 + O \leftrightarrow HCO + H$	6.00E+12	0	0
222	$CH_2 + H \leftrightarrow CH + H_2$	4.30E+10	−1800	0
223	$CH_2 + O_2 \leftrightarrow HCO + OH$	6.90E+11	−500	0
224	$CH_2 + O_2 \leftrightarrow CO_2 + H_2$	1.60E+12	500	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
225	$CH_2 + O_2 \leftrightarrow CO_2 + H + H$	1.90E + 10	1000	0
226	$CH_2 + O_2 \leftrightarrow CO + H_2O$	8.60E + 10	−1000	0
227	$CH_2 + O_2 \leftrightarrow CO + OH + H$	5.00E + 13	−500	0
228	$CH_2 + O_2 \leftrightarrow CH_2O + O$	1.10E + 11	9000	0
229	$CH_2 + CO_2 \leftrightarrow CH_2O + CO$	1.20E + 13	1000	0
230	$CH_2 + CH_2 \leftrightarrow C_2H_2 + H_2$	1.20E + 14	800	0
231	$CH_2 + CH_2 \leftrightarrow C_2H_2 + H + H$	4.20E + 13	800	0
232	$CH_2 + CH_3 \leftrightarrow C_2H_4 + H$	4.00E + 13	0	0
233	$CH_2 + CH \leftrightarrow C_2H_2 + H$	1.60E + 14	0	0
234	$CH_2 + M \leftrightarrow C + H_2 + M$	6.00E + 12	64000	0
235	$SCH_2 + M \leftrightarrow CH_2 + M$	3.00E + 13	0	0
236	$SCH_2 + O_2 \leftrightarrow CO + OH + H$	3.00E + 13	0	0
237	$SCH_2 + H \leftrightarrow CH + H_2$	1.50E + 13	0	0
238	$SCH_2 + O \leftrightarrow CO + H + H$	1.50E + 13	0	0
239	$SCH_2 + O \leftrightarrow CO + H_2$	3.00E + 13	0	0
240	$SCH_2 + OH \leftrightarrow CH_2O + H$	3.00E + 13	0	0
241	$SCH_2 + HO_2 \leftrightarrow CH_2O + OH$	3.00E + 13	0	0
242	$SCH_2 + H_2O_2 \leftrightarrow CH_3O + OH$	1.80E + 13	0	0
243	$SCH_2 + H_2O \leftrightarrow\leftrightarrow > CH_3OH$	1.20E + 12	0	0
244	$SCH_2 + CH_2O \leftrightarrow CH_3 + HCO$	1.80E + 13	0	0
245	$SCH_2 + HCO \leftrightarrow CH_3 + CO$	1.80E + 13	0	0
246	$SCH_2 + CH_3 \leftrightarrow C_2H_4 + H$	4.00E + 13	0	0
247	$SCH_2 + CH_4 \leftrightarrow CH_3 + CH_3$	1.20E + 14	0	0
248	$SCH_2 + C_2H_6 \leftrightarrow CH_3 + C_2H_5$	3.00E + 12	0	0
249	$SCH_2 + CO_2 \leftrightarrow CH_2O + CO$	1.60E + 14	0	0
250	$SCH_2 + CH_2CO \leftrightarrow C_2H_4 + CO$	3.00E + 13	0	0
251	$CH + OH \leftrightarrow HCO + H$	4.00E + 13	0	0
252	$CH + O \leftrightarrow CO + H$	4.90E + 13	0	0
253	$CH + O_2 \leftrightarrow HCO + O$	4.90E + 13	0	0
254	$CH + O_2 \leftrightarrow CO + OH$	3.40E + 12	0	0
255	$CH + CO_2 \leftrightarrow HCO + CO$	3.00E + 13	690	0
256	$CH + CH_4 \leftrightarrow C_2H_4 + H$	3.00E + 13	−400	0
257	$CH + CH_3 \leftrightarrow C_2H_3 + H$	1.13E + 07	0	0
258	$CH_2 + OH \leftrightarrow CH + H_2O$	7.80E + 13	3000	2
259	$CH + H \leftrightarrow C + H_2$	1.17E + 15	0	0
260	$CH + H_2O \leftrightarrow CH_2O + H$	1.00E + 14	0	−0.75
261	$CH + CH_2O \leftrightarrow CH_2CO + H$	5.40E + 13	−515	0
262	$CH_3O + M \leftrightarrow CH_2O + H + M$	3.00E + 11	13500	0
263	$CH_3O + HO_2 \leftrightarrow CH_2O + H_2O2$	1.00E + 13	0	0
264	$CH_3O + OH \leftrightarrow CH_2O + H_2O$	1.80E + 12	0	0
265	$CH_3O + O \leftrightarrow CH_2O + OH$	1.80E + 13	0	0
266	$CH_3O + H \leftrightarrow CH_2O + H_2$	2.20E + 10	0	0
267	$CH_3O + O_2 \leftrightarrow CH_2O + HO_2$	1.15E + 11	1750	0
268	$CH_3O + CH_2O \leftrightarrow CH_3OH + HCO$	1.57E + 13	1280	0
269	$CH_3O + CO \leftrightarrow CH_3 + CO_2$	9.00E + 13	11804	0
270	$CH_3O + HCO \leftrightarrow CH_3OH + CO$	2.41E + 13	0	0
271	$CH_3O + C_2H_5 \leftrightarrow CH_2O + C_2H_6$	2.41E + 13	0	0
272	$CH_3O + C_2H_3 \leftrightarrow CH_2O + C_2H_4$	1.20E + 11	0	0
273	$CH_3O + C_2H_4 \leftrightarrow CH_2O + C_2H_5$	3.40E + 06	6750	0
274	$CH_3O + H \leftrightarrow CH_2OH + H$	1.00E + 12	0	1.6
275	$CH_3O + H \leftrightarrow SCH_2 + H_2O$	5.00E + 35	0	0
276	$CH_2O + M \leftrightarrow HCO + H + M$	1.10E + 36	96680	−5.54
277	$CH_2O + M \leftrightarrow CO + H_2 + M$	3.00E + 12	96680	−5.54
278	$CH_2O + HO_2 \leftrightarrow HCO + H_2O_2$	3.43E + 09	13000	0
279	$CH_2O + OH \leftrightarrow HCO + H_2O$	4.10E + 11	−447	1.18
280	$CH_2O + O \leftrightarrow HCO + OH$	1.26E + 08	2760	0.57
281	$CH_2O + H \leftrightarrow HCO + H_2$	6.00E + 13	2166	1.62
282	$CH_2O + O_2 \leftrightarrow HCO + HO_2$	7.80E-08	40650	0
283	$CH_2O + CH_3 \leftrightarrow HCO + CH_4$	8.85E + 20	1970	6.1
284	$C_2H_6 + M \leftrightarrow C_2H_5 + H$	1.33E + 13	102210	−1.228
285	$C_2H_6 + HO_2 \leftrightarrow C_2H5 + H_2O_2$	7.20E + 06	20535	0
286	$C_2H_6 + OH \leftrightarrow C_2H_5 + H_2O$	1.00E + 09	870	2
287	$C_2H_6 + O \leftrightarrow C_2H_5 + OH$	1.40E + 09	5800	1.5
288	$C_2H_6 + H \leftrightarrow C_2H_5 + H_2$	6.00E + 13	7400	1.5
289	$C_2H_6 + O_2 \leftrightarrow C_2H_5 + HO_2$	1.47E-07	52000	0
290	$C_2H_6 + CH_3 \leftrightarrow C_2H_5 + CH_4$	6.50E + 12	6060	6
291	$C_2H_6 + CH_2 \leftrightarrow CH_3 + C_2H_5$	8.57E-02	7911	0
292	$C_2H_6 + C_2H_3 \leftrightarrow C_2H_4 + C_2H_5$	4.70E + 04	2543	4.14
293	$C_2H_6 + HCO \leftrightarrow CH_2O + C_2H_5$	1.11E + 10	18235	2.72
294	$C_2H_5 + M \leftrightarrow C_2H_4 + H$	8.20E + 13	36767	1.037
295	$C_2H_5 + M \leftrightarrow C_2H_4 + H$	3.00E + 11	39880	0
296	$C_2H_5 + HO_2 \leftrightarrow C_2H_4 + H_2O_2$	2.41E + 13	0	0
297	$C_2H_5 + OH \leftrightarrow C_2H_4 + H_2O$	2.41E + 13	0	0
298	$C_2H_5 + OH \rightarrow CH_3 + CH_2O + H$	4.24E + 13	0	0
299	$C_2H_5 + O \leftrightarrow CH_2O + CH_3$	5.30E + 13	0	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
300	$C_2H_5 + O \leftrightarrow CH_3HCO + H$	3.46E + 13	0	0
301	$C_2H_5 + O \leftrightarrow C_2H_4 + OH$	1.25E + 14	0	0
302	$C_2H_5 + H \leftrightarrow C_2H_4 + H_2$	1.00E + 10	8000	0
303	$C_2H_5 + O2 \leftrightarrow C_2H_4 + HO_2$	1.10E + 12	−2200	0
304	$C_2H_5 + CH3 \leftrightarrow C_2H_4 + CH_4$	1.40E + 12	0	0
305	$C_2H_5 + C2H5 \leftrightarrow C_2H_4 + C_2H_6$	2.50E + 13	0	0
306	$C_2H_5 + HO2 \leftrightarrow\leftrightarrow > CH_3 + CH_2O + OH$	3.00E + 13	0	0
307	$C_2H_5 + HO_2 \leftrightarrow C_2H_5O + OH$	3.50E + 16	0	0
308	$C_2H_4 + M \leftrightarrow C_2H_2 + H_2 + M$	2.60E + 17	71530	0
309	$C_2H_4 + M \leftrightarrow C_2H_3 + H + M$	5.53E + 05	96570	0
310	$C_2H_4 + OH \leftrightarrow C_2H_3 + H_2O$	8.10E + 06	2900	2.31
311	$C_2H_4 + O \leftrightarrow CH_3 + HCO$	4.49E + 07	180	1.88
312	$C_2H_4 + H \leftrightarrow C_2H_3 + H_2$	4.00E + 13	13366	2.12
313	$C_2H_4 + O_2 \leftrightarrow C_2H_3 + HO_2$	1.86E + 14	61500	0
314	$C_2H_4 + C_2H_4 \leftrightarrow C_2H_5 + C_2H_3$	4.20E + 12	64200	0
315	$C_2H_4 + CH_3 \leftrightarrow C_2H_3 + CH_4$	4.70E + 06	11100	0
316	$C_2H_4 + O \leftrightarrow CH_2HCO + H$	3.00E + 04	180	1.88
317	$C_2H_4 + O \leftrightarrow CH_2O + CH_2$	6.70E + 05	180	1.88
318	$C_2H_4 + O \leftrightarrow CH_2CO + H_2$	1.51E + 07	180	1.88
319	$C_2H_4 + O \leftrightarrow C_2H_3 + OH$	2.00E + 12	3790	1.91
320	$C_2H_4 + OH \leftrightarrow CH_2O + CH_3$	5.42E + 12	960	0
321	$C_2H_4 + OH + M \leftrightarrow PC_2H_5O$	1.12E + 13	0	0
322	$C_2H_4 + HO_2 \leftrightarrow C2H3 + H2O2$	1.00E + 11	30400	0
323	$C_2H_4 + CH_3O \leftrightarrow C_2H_3 + CH_3OH$	2.10E + 14	10000	0
324	$C_2H_3 + M \leftrightarrow C_2H_2 + H$	3.00E + 13	39740	0
325	$C_2H_3 + HO_2 \leftrightarrow\leftrightarrow > CH_3 + CO + OH$	3.00E + 13	0	0
326	$C_2H_3 + OH \leftrightarrow C_2H_2 + H2O$	1.20E + 13	0	0
327	$C_2H_3 + H \leftrightarrow C_2H_2 + H_2$	1.00E + 13	0	0
328	$C_2H_3 + O \leftrightarrow CH_3 + CO$	1.70E + 29	0	0
329	$C_2H_3 + O_2 \leftrightarrow CH_2O + HCO$	5.00E + 13	6500	−5.312
330	$C_2H_3 + CH \leftrightarrow CH_2 + C_2H_2$	3.92E + 11	0	0
331	$C_2H_3 + CH_3 \leftrightarrow C_2H_2 + CH_4$	3.00E + 13	0	0
332	$C_2H_3 + C_2H \leftrightarrow C_2H_2 + C_2H_2$	9.03E + 13	0	0
333	$C_2H_3 + HCO \leftrightarrow C_2H_4 + CO$	5420	0	0
334	$C_2H_3 + CH_2O \leftrightarrow C_2H_4 + HCO$	1.45E + 13	5862	2.81
335	$C_2H_3 + C_2H_3 \leftrightarrow C_2H_2 + C_2H_4$	1.00E + 13	0	0
336	$C_2H_33 + O \leftrightarrow C_2H_2 + OH$	1.00E + 13	0	0
337	$C_2H_3 + O \leftrightarrow CH_2 + HCO$	1.00E + 13	0	0
338	$C_2H_3 + O \leftrightarrow CH_2CO + H$	3.00E + 13	0	0
339	$C_2H_3 + OH \leftrightarrow CH_3HCO$	5.19E + 15	0	0
340	$C_2H_3 + O_2 \leftrightarrow C_2H_2 + HO_2$	2.12E-06	3310	−1.26
341	$C_2H_3 + O_2 \leftrightarrow C_2H_2 + HO2$	3.50E + 14	9484	6
342	$C_2H_3 + O_2 \leftrightarrow CH_2HCO + O$	3.00E + 13	5260	−0.61
343	$C_2H_3 + CH_2 \leftrightarrow C_2H_2 + CH_3$	2.37E + 32	0	0
344	$C_2H_2 \leftrightarrow C_2H + H$	2.00E + 08	130688	−5.28
345	$C_2H_2 + O_2 \leftrightarrow HCCO + OH$	1.20E + 13	30100	1.5
346	$C_2H_2 + O_2 \leftrightarrow C_2H + HO_2$	3.39E + 07	74520	0
347	$C_2H_2 + OH \leftrightarrow C_2H + H_2O$	2.18E-04	14000	2
348	$C_2H_2 + OH \leftrightarrow CH_2CO + H$	1.20E + 06	−1000	4.5
349	$C_2H_2 + O \leftrightarrow CH_2 + CO$	5.00E + 06	1570	2.1
350	$C_2H_2 + O \leftrightarrow HCCO + H$	1.80E + 11	1570	2.1
351	$C_2H_2 + CH_3 \leftrightarrow C_2H + CH_4$	3.00E + 14	17290	0
352	$C_2H_2 + O \leftrightarrow C_2H + OH$	4.83E-04	25000	0
353	$C_2H_2 + OH \leftrightarrow CH_3 + CO$	6.10E + 09	−2000	4
354	$C_2H_2 + HO_2 \leftrightarrow CH_2CO + OH$	4.00E + 12	7950	0
355	$C_2H_2 + O_2 \leftrightarrow HCO + HCO$	2.00E + 13	28000	0
356	$C_2H + OH \leftrightarrow HCCO + H$	4.00E + 07	0	0
357	$C_2H + OH \leftrightarrow C_2 + H_2O$	1.00E + 13	8000	2
358	$C_2H + O \leftrightarrow CO + CH$	9.00E + 12	0	0
359	$C_2H + O_2 \leftrightarrow HCO + CO$	1.10E + 13	0	0
360	$C_2H + H_2 \leftrightarrow C_2H_2 + H$	9.00E + 12	2165	0
361	$C_2H + O_2 \leftrightarrow CO + CO + H$	6.00E + 11	0	0
362	$C_2H + O_2 \leftrightarrow HCCO + O$	3.00E + 14	0	0
363	$CH_2CO + M \leftrightarrow CH_2 + CO$	2.00E + 13	71000	0
364	$CH_2CO + O_2 \leftrightarrow CH_2O + CO_2$	6.00E + 11	61500	0
365	$CH_2CO + HO \rightarrow CH_2O + CO + OH$	1.00E + 13	12738	0
366	$CH_2CO + O \leftrightarrow HCCO + OH$	1.00E + 13	8000	0
367	$CH_2CO + OH \leftrightarrow CH_2OH + CO$	1.80E + 13	0	0
368	$CH_2CO + H \leftrightarrow CH_3 + CO$	2.40E + 12	3400	0
369	$CH_2CO + CH_3 \leftrightarrow C_2H_5 + CO$	1.00E + 12	8000	0
370	$CH_2CO + CH_2 \leftrightarrow C_2H_4 + CO$	3.60E + 13	0	0
371	$CH_2CO + CH_2 \leftrightarrow HCCO + CH_3$	7.50E + 12	11000	0
372	$CH_2CO + CH_3 \leftrightarrow HCCO + CH_4$	2.80E + 13	13000	0
373	$CH_2CO + OH \leftrightarrow CH_2O + HCO$	5.00E + 13	0	0
374	$CH_2CO + H \leftrightarrow HCCO + H_2$	7.50E + 11	8000	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
375	$CH_2CO + O \leftrightarrow HCO + HCO$	7.50E+11	1350	0
376	$CH_2CO + O \leftrightarrow HCO + CO + H$	7.50E+11	1350	0
377	$CH_2CO + O \leftrightarrow CH_2O + CO$	7.50E+12	1350	0
378	$CH_2CO + OH \leftrightarrow HCCO + H_2O$	6.00E+15	2000	0
379	$HCCO + M \leftrightarrow CH + CO + M$	1.00E+13	58821	0
380	$HCCO + OH \leftrightarrow HCO + CO + H$	3.00E+13	0	0
381	$HCCO + OH \leftrightarrow C_2O + H_2O$	1.00E+14	0	0
382	$HCCO + O \leftrightarrow CO + CO + H$	1.50E+14	0	0
383	$HCCO + H \leftrightarrow CH_2 + CO$	5.40E+11	0	0
384	$HCCO + O_2 \leftrightarrow CO_2 + CO + H$	1.00E+13	850	0
385	$HCCO + CH_2 \leftrightarrow C_2H + CH_2O$	3.00E+13	2000	0
386	$HCCO + CH_2 \leftrightarrow C_2H_3 + CO$	2.00E+12	0	0
387	$HCCO + CH_3 \leftrightarrow C_2H_4 + CO$	5.00E+13	0	0
388	$HCCO + CH \leftrightarrow CO + C_2H_2$	1.00E+13	0	0
389	$HCCO + HCCO \leftrightarrow CO + C_2H_2 + CO$	1.00E+13	0	0
390	$HCCO + OH \leftrightarrow HCO + HCO$	5.40E+11	0	0
391	$HCCO + O_2 \leftrightarrow CO + CO + OH$	5.40E+11	850	0
392	$HCCO + O_2 \leftrightarrow CO_2 + HCO$	1.70E+16	850	0
393	$CH_3OH + M \leftrightarrow CH_3 + OH$	6.30E+12	90885	0
394	$CH_3OH + HO_2 \leftrightarrow CH_2OH + H_2O_2$	3.00E+04	19360	0
395	$CH_3OH + OH \leftrightarrow CH_2OH + H_2O$	5300	−883	2.65
396	$CH_3OH + OH \leftrightarrow CH_3O + H_2O$	3.88E+05	−883	2.65
397	$CH_3OH + O \leftrightarrow CH_2OH + OH$	3.20E+13	3080	2.5
398	$CH_3OH + H \leftrightarrow CH_2OH + H_2$	3.19E+01	6095	0
399	$CH_3OH + CH_3 \leftrightarrow CH_2OH + CH_4$	1.45E+01	7172	3.17
400	$CH_3OH + CH_3 \leftrightarrow CH_3O + CH_4$	1.44E+01	6935	3.1
401	$CH_3OH + C_2H_5 \leftrightarrow C_2H_6 + CH_3O$	8.00E+10	8942	3.1
402	$CH_3OH + H \leftrightarrow CH_3 + H_2O$	1.30E+05	0	0
403	$CH_3OH + O \leftrightarrow CH_3O + OH$	2.00E+12	5000	2.5
404	$CH_3OH + CH_3 \leftrightarrow C_2H_6 + OH$	1.50E+12	15000	0
405	$CH_3OH + CH_3O \leftrightarrow CH_2OH + CH_3OH$	1.38E+16	7000	0
406	$CH_3OH + M \leftrightarrow CH_2OH + H$	8.00E+12	95950	0
407	$CH_3OH + H \leftrightarrow H_2 + CH_3O$	2.05E+13	6095	0
408	$CH_3OH + O2 \leftrightarrow CH_2OH + HO_2$	3.19E+01	44900	0
409	$CH_3OH + C_2H_5 \leftrightarrow C_2H_6 + CH_2OH$	1.14E+43	9161	3.2
410	$CH_2OH + M \leftrightarrow CH_2O + H + M$	3.00E+13	43000	-8
411	$CH_2OH + H \leftrightarrow CH_2O + H_2$	1.50E+15	0	0
412	$CH_2OH + O_2 \leftrightarrow CH_2O + HO_2$	7.20E+13	0	−1
413	$CH_2OH + O_2 \leftrightarrow CH_2O + HO_2$	1.00E+12	3570	0
414	$H + CH_2OH \leftrightarrow SCH_2 + H_2O$	1.00E+13	0	0
415	$CH_2OH + O \leftrightarrow CH_2O + OH$	1.00E+13	0	0
416	$CH_2OH + OH \leftrightarrow CH_2O + H_2O$	1.21E+13	0	0
417	$CH_2OH + HO_2 \leftrightarrow CH_2O + H_2O_2$	2.82E+12	0	0
418	$CH_2OH + CH_2OH \leftrightarrow CH_3OH + CH_2O$	1.00E+15	0	0
419	$CH_2OH + CH_2OH \leftrightarrow CH_2O + CH_2O + H_2$	1.21E+14	0	−0.7
420	$CH_2OH + HCO \leftrightarrow CH_3OH + CO$	5490	0	0
421	$CH_2OH + CH_2O \leftrightarrow CH_3OH + HCO$	2.40E+13	5900	2.8
422	$CH_2OH + CH_3O \leftrightarrow CH_3OH + CH_2O$	2.32E+13	0	0
423	$CH_3O + CH_3O \leftrightarrow CH_3OH + CH_2O$	7.10E+15	0	0
424	$CH_3HCO \leftrightarrow CH_3 + HCO$	3.00E+12	81790	0
425	$CH_3HCO + HO_2 \leftrightarrow CH_3CO + H_2O_2$	2.30E+10	12000	0
426	$CH_3HCO + OH \leftrightarrow CH_3CO + H_2O$	5.80E+12	−1100	0.73
427	$CH_3HCO + O \leftrightarrow CH_3CO + OH$	4.10E+09	1800	0
428	$CH_3HCO + H \leftrightarrow CH_3CO + H_2$	3.00E+13	2400	1.16
429	$CH_3HCO + O_2 \leftrightarrow CH_3CO + HO_2$	7.60E+00	39200	0
430	$CH_3HCO + CH_3 \leftrightarrow CH_3CO + CH_4$	7.00E+08	3740	3.4
431	$CH_3HCO + H \leftrightarrow CH_2HCO + H_2$	5.00E+08	7400	1.5
432	$CH_3HCO + O \leftrightarrow CH_2HCO + OH$	2.00E+14	5800	1.5
433	$CH_3HCO + OH \leftrightarrow CH_2HCO + H_2O$	3.00E+13	6000	0
434	$CH_3HCO + HO_2 \leftrightarrow CH_2HCO + H_2O_2$	1.66E+12	15000	0
435	$CH_3HCO + CH_2 \leftrightarrow CH_3CO + CH_3$	1.58E+00	3510	0
436	$CH_3HCO + CH_3 \leftrightarrow CH_2HCO + CH_4$	5.00E+12	7720	4
437	$CH_3HCO + CH_3O \leftrightarrow CH_3CO + CH_3OH$	1.26E+12	0	0
438	$CH_3HCO + C_2H_5 \leftrightarrow CH_3CO + C_2H_6$	8.13E+10	8500	0
439	$CH_3HCO + C_2H_3 \leftrightarrow CH_3CO + C_2H_4$	1.60E+11	3680	0
440	$CH_2HCO \leftrightarrow CH_3CO$	3.00E+12	21600	0
441	$CH_3HCO + CH_2HCO \leftrightarrow CH_3CO + CH_3HCO$	2.80E+13	11200	0
442	$CH_3CO + M \leftrightarrow CH_3 + CO$	3.30E+13	17150	0
443	$CH_3CO + H \leftrightarrow CH_2CO + H_2$	4.00E+13	0	0
444	$CH_3CO + O \leftrightarrow CH_2CO + OH$	1.50E+14	0	0
445	$CH_3CO + O \leftrightarrow CH_3 + CO_2$	3.30E+13	0	0
446	$CH_3CO + CH_3 \leftrightarrow C_2H_6 + CO$	2.00E+13	0	0
447	$CH2HCO + H \leftrightarrow CH2CO + H2$	2.00E+10	0	0
448	$CH2HCO + O2 \rightarrow CH2O + OH + CO$	1.50E+11	0	0
449	$CH2HCO + O2 \leftrightarrow CH2CO + HO2$	1.58E+13	0	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
450	CH2HCO↔CH2CO + H	1.00E + 15	35200	0
451	C2H5O↔CH3 + CH2O	9.77E + 10	21600	0
452	C2H5O + O2↔CH3HCO + HO2	2.00E + 14	1590	0
453	C2H5O↔CH3HCO + H	1.00E + 14	23300	0
454	C2H5O + OH↔CH3HCO + H2O	1.00E + 14	0	0
455	C2H5O + H↔CH3HCO + H2	1.21E + 14	0	0
456	C2H5O + O↔CH3HCO + OH	1.00E + 14	0	0
457	C2H5O + HO2↔CH3HCO + H2O2	5.00E + 13	0	0
458	SC2H5O + M↔CH3HCO + H + M	2.00E + 13	21860	0
459	SC2H5O + H↔CH3HCO + H2	1.50E + 13	0	0
460	SC2H5O + OH↔CH3HCO + H2O	9.04E + 13	0	0
461	SC2H5O + O↔CH3HCO + OH	8.40E + 15	0	0
462	SC2H5O + O2↔CH3HCO + HO2	4.80E + 14	0	−1.2
463	SC2H5O + O2↔CH3HCO + HO2	1.00E + 13	5000	0
464	SC2H5O + HO2→CH3HCO + OH + OH	1.00E + 11	0	0
465	PC2H5O↔SC2H5O	3.10E + 15	27000	0
466	C2H5OH↔CH2OH + CH3	8.00E + 06	80600	0
467	C2H5OH + OH↔SC2H5O + H2O	1.14E + 06	−1541	1.776
468	C2H5OH + OH↔C2H5O + H2O	2.56E + 06	914	2
469	C2H5OH + OH↔PC2H5O + H2O	6.00E + 05	860	2.06
470	C2H5OH + O↔SC2H5O + OH	4.82E + 13	1850	2.46
471	C2H5OH + O↔C2H5O + OH	5.00E + 12	6856	0
472	C2H5OH + O↔PC2H5O + OH	2.40E + 10	4411	0
473	C2H5OH + H→C2H5 + H2O	4.40E + 12	0	0
474	C2H5OH + H↔SC2H5O + H2	2.00E + 13	4570	0
475	C2H5OH + HO2↔SC2H5O + H2O2	4.00E + 11	17000	0
476	C2H5OH + CH3↔SC2H5O + CH4	3	9700	0
477	C2H5OH + CH3↔PC2H5O + CH4	8.00E + 10	10480	4
478	C2H5OH + CH3↔C2H5O + CH4	2.00E + 11	9400	0
479	C2H5OH + CH3O↔SC2H5O + CH3OH	1.50E + 12	7000	0
480	C2H5OH + CH2O↔C2H5O + CH3O	2.00E + 11	79500	0
481	C2H5OH + C2H5O↔C2H5OH + SC2H5O	5.00E + 16	7000	0
482	C2H5OH↔C2H5 + OH	1.00E + 14	91212	0
483	C2H5OH↔C2H4 + H2O	4.00E + 13	76706	0
484	C2H5OH + O2↔PC2H5O + HO2	4.00E + 13	50900	0
485	C2H5OH + O2↔SC2H5O + HO2	2.00E + 13	51200	0
486	C2H5OH + O2↔C2H5O + HO2	2.00E + 12	56000	0
487	C2H5OH + H↔PC2H5O + H2	1.76E + 12	9500	0
488	C2H5OH + H↔C2H5O + H2	1.00E + 11	4570	0
489	C2H5OH + HO2↔H2O2 + C2H5O	1.00E + 11	15500	0
490	C2H5OH + HO2↔H2O2 + PC2H5O	1.50E + 12	12500	0
491	C2H5OH + C2H5↔PC2H5O + C2H6	4.00E + 13	11700	0
492	C2H5OH + C2H5↔SC2H5O + C2H6	4.00E + 11	10000	0
493	C2H5OH + CH2OH↔SC2H5O + CH3OH	5.00E + 13	9700	0
494	C + OH↔CO + H	2.00E + 13	0	0
495	C + O2↔CO + O	5.00E + 13	0	0
496	C + CH3↔C2H2 + H	5.00E + 13	0	0
497	C + CH2↔C2H + H	1.30E + 11	0	0
498	CH2O + CH3O2↔HCO + CH3O2H	2.40E + 13	9000	0
499	CH3O2 + CH3↔CH3O + CH3O	2.70E + 10	0	0
500	CH3O2 + CH3O2→CH2O + CH3OH + O2	2.80E + 10	−780	0
501	CH3O2 + CH3O2→CH3O + CH3O + O2	2.40E + 12	−780	0
502	CH3O2 + H2O2↔CH3O2H + HO2	6.00E + 14	10000	0
503	CH3O2H↔CH3O + OH	2.50E + 11	42300	0
504	CH3O2 + HO2↔CH3O2H + O2	7.20E + 11	−1570	0
505	CH3O2H + OH↔CH3O2 + H2O	1.81E + 11	−250	0
506	CH4 + CH3O2↔CH3 + CH3O2H	1.81E + 12	18600	0
507	CH3OH + CH3O2↔CH2OH + CH3O2H	2.00E + 13	13800	0
508	CH3O2H + O↔OH + CH3O2	1.00E + 10	4750	0
509	CH3CO + O2↔CH3CO3	1.20E + 11	−2700	0
510	CH3HCO + CH3CO3↔CH3CO + CH3CO3H	1.15E + 11	4900	0
511	CH3HCO + C2H5O2↔CH3CO + C2H5O2H	7.94E + 11	10000	0
512	C2H5 + O2↔C2H5O2	5.62E + 11	−840	0
513	C2H5O2↔C2H4 + HO2	3.40E + 11	28900	0
514	C2H5O2 + HO2↔C2H5O2H + O2	4.00E + 15	−1300	0
515	C2H5O2H↔C2H5O + OH	2.00E + 13	43000	0
516	C2H5O2H + O↔OH + C2H5O2	2.00E + 12	4750	0
517	C2H5O2H + OH↔C2H5O2 + H2O	1.14E + 13	−370	0
518	CH4 + C2H5O2↔CH3 + C2H5O2H	1.14E + 13	20460	0
519	CH4 + CH3CO3↔CH3 + CH3CO3H	1.00E + 12	20460	0
520	C2H4 + C2H5O2↔C2H3 + C2H5O2H	3.00E + 12	25000	0
521	C2H4 + CH3CO3↔C2H3 + CH3CO3H	1.00E + 12	29000	0
522	CH3CO3 + HO2↔CH3CO3H + O2	1.15E + 13	0	0
523	CH3CO3H→CH3CO2 + OH	2.00E + 14	32550	0
524	CH3CO3H→CH3 + CO2 + OH	1.08E + 15	40150	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
525	CH3CO3 + CH3O2→CH3CO2 + CH3O + O2	2.47E + 09	3600	0
526	CH3CO3 + CH3O2→ > CH3CO2H + CH2O + O2	2.59E + 11	− 4200	0
527	CH3CO3 + HO2→CH3CO2 + OH + O2	1.69E + 12	− 2080	0
528	CH3CO3 + CH3CO3→CH3CO2 + CH3CO2 + O2	8.70E + 15	− 1060	0
529	CH3CO2 + M→CH3 + CO2 + M	6.30E + 12	14400	0
530	CH3OH + C2H5O2↔CH2OH + C2H5O2H	6.30E + 12	19360	0
531	CH3OH + CH3CO3↔CH2OH + CH3CO3H	1.30E + 11	19360	0
532	CH2O + C2H5O2↔HCO + C2H5O2H	1.00E + 12	9000	0
533	CH2O + CH3CO3↔HCO + CH3CO3H	1.00E + 13	10560	0
534	C2H4 + CH3O2↔C2H3 + CH3O2H	1.15E + 11	25000	0
535	CH3HCO + CH3O2↔CH3CO + CH3O2H	1.00E + 13	10000	0
536	C2H5OH + CH3O2↔SC2H5O + CH3O2H	2.41E + 13	10000	0
537	C2H5 + CH3O2↔C2H5O + CH3O	2.20E + 12	0	0
538	C2H4 + HO2↔C2H4O + OH	1.00E + 11	17200	0
539	C2H4 + CH3O↔C2H4O + CH3	7.00E + 11	14500	0
540	C2H4 + CH3O2↔C2H4O + CH3O	1.60E + 13	14500	0
541	C2H4O→CH3HCOW	1.00E + 14	54300	0
542	CH3HCOW + M→CH3HCO + M	5.00E + 08	0	0
543	CH3HCOW→CH3 + HCO	8.00E + 13	0	0
544	C2H4O + H↔H2 + C2H3O	5.00E + 09	9740	0
545	C2H4O + H↔H2O + C2H3	9.51E + 10	5030	0
546	C2H4O + H↔C2H4 + OH	1.00E + 11	5030	0
547	C2H4O + CH2HCO↔CH3HCO + C2H3O	1.07E + 12	14000	0
548	C2H4O + CH3↔CH4 + C2H3O	1.91E + 12	11900	0
549	C2H4O + O↔OH + C2H3O	1.78E + 13	5300	0
550	C2H4O + OH↔H2O + C2H3O	1.00E + 11	3600	0
551	C2H3O→CH2CHOW	8.00E + 11	10000	0
552	C2H3O→CH3 + CO	4.00E + 15	10000	0
553	C2H3O + H + M→C2H4O + M	1.00E + 14	0	0
554	CH2CHOW + M→CH2HCO + M	1.00E + 08	0	0
555	CH2CHOW→CH3 + CO	1.00E + 11	0	0
556	CH2CHOW→OH + C2H2	1.00E + 08	17000	0
557	CH2CHOW→CH2CO + H	1.00E + 14	0	0
558	C2H4O + O2↔HO2 + C2H3O	5.00E + 13	52000	0
559	C2H4O + HO2↔H2O2 + C2H3O	1.00E + 14	18000	0
560	CH3HCOW + O2→HO2 + CH3CO	1.00E + 14	0	0
561	CH2CHOW + O2→HO2 + CH2CO	1.20E + 13	0	0
562	CH2 + C2H2↔H + C3H3	3.16E + 12	6620	0
563	CH2 + C2H4↔C3H6	1.00E + 14	5280	0
564	SCH2 + C2H4→C3H6	2.19E + 12	0	0
565	CH2 + C3H8↔CH3 + IC3H7	1.79E + 12	6405	0
566	CH2 + C3H8↔CH3 + NC3H7	1.80E + 14	6405	0
567	SCH2 + C2H2↔C3H3 + H	3.00E + 13	0	0
568	C2H3 + CH2↔C3H4 + H	2.00E + 12	0	0
569	C2H3 + C2H2↔C4H4 + H	7.23E + 13	5000	0
570	C2H3 + C2H3↔C4H6	1.61E + 40	0	0
571	C2H2 + CH3↔SC3H5	2.61E + 46	20331	− 8.58
572	C2H2 + CH3↔C3H5	6.74E + 19	36951	− 9.82
573	C2H2 + CH3↔C3H4 + H	1.00E + 12	31591	− 2.08
574	CH2CO + C2H3↔C3H5 + CO	1.00E + 11	3000	0
575	HCCO + C2H2↔C3H3 + CO	2.09E + 88	3000	0
576	C3H8↔C2H5 + CH3	4.00E + 13	126100	− 20.9
577	C3H8 + O2↔NC3H7 + HO2	4.00E + 13	50870	0
578	C3H8 + O2↔IC3H7 + HO2	9.52E + 04	47690	0
579	C3H8 + HO2↔NC3H7 + H2O2	1.93E + 04	16494	2.55
580	C3H8 + HO2↔IC3H7 + H2O2	3.16E + 07	13910	2.6
581	C3H8 + OH↔NC3H7 + H2O	7.06E + 06	934	1.8
582	C3H8 + OH↔IC3H7 + H2O	3.72E + 06	− 159	1.9
583	C3H8 + O↔NC3H7 + OH	5.50E + 05	5505	2.4
584	C3H8 + O↔IC3H7 + OH	1.34E + 06	3140	2.5
585	C3H8 + H↔NC3H7 + H2	1.30E + 06	6756	2.54
586	C3H8 + H↔IC3H7 + H2	3.00E + 12	4470	2.4
587	C3H8 + CH3↔NC3H7 + CH4	8.07E + 11	11710	0
588	C3H8 + CH3↔IC3H7 + CH4	3.16E + 11	10110	0
589	C3H8 + C2H5↔NC3H7 + C2H6	5.01E + 10	12300	0
590	C3H8 + C2H5↔IC3H7 + C2H6	600	10400	0
591	C3H8 + C2H3↔NC3H7 + C2H4	1000	10502	3.3
592	C3H8 + C2H3↔IC3H7 + C2H4	1.00E + 11	8829	3.1
593	C3H8 + IC3H7↔NC3H7 + C3H8	7.94E + 11	12900	0
594	C3H8 + C3H5↔NC3H7 + C3H6	7.94E + 11	20500	0
595	C3H8 + C3H5↔IC3H7 + C3H6	3.18E + 11	16200	0
596	C3H8 + CH3O↔NC3H7 + CH3OH	7.20E + 10	7050	0
597	C3H8 + CH3O↔IC3H7 + CH3OH	1.26E + 13	4470	0
598	NC3H7↔C2H4 + CH3	3.58E + 09	30404	0
599	NC3H7 + O2↔C3H6 + HO2	1.00E + 14	− 3532	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
600	IC3H7↔C2H4 + CH3	2.75E + 10	45000	0
601	IC3H7 + O2↔C3H6 + HO2	4.57E + 14	− 2151	0
602	C3H6↔C3H5 + H	7.59E + 14	88900	0
603	C3H6↔SC3H5 + H	1.45E + 15	101300	0
604	C3H6↔TC3H5 + H	1.10E + 21	98060	0
605	C3H6↔C2H3 + CH3	1.02E + 12	97720	− 1.2
606	C3H6 + HO2↔C3H6O + OH	1.50E + 11	14964	0
607	C3H6 + HO2↔C3H5 + H2O2	9640	14190	0
608	C3H6 + HO2↔SC3H5 + H2O2	9640	13910	2.6
609	C3H6 + HO2↔TC3H5 + H2O2	9.98E + 12	13910	2.6
610	C3H6 + OH↔C3H5 + H2O	4.99E + 12	3060	0
611	C3H6 + OH↔SC3H5 + H2O	4.99E + 12	3060	0
612	C3H6 + OH↔TC3H5 + H2O	6.83E + 06	3060	0
613	C3H6 + O↔C2H5 + HCO	9.11E + 06	− 628	1.57
614	C3H6 + O↔CH3 + CH3CO	4.56E + 06	− 628	1.57
615	C3H6 + O↔C2H4 + CH2O	1.00E + 14	− 628	1.57
616	NC3H7↔C3H6 + H	5.70E + 09	37286	0
617	C3H6 + H↔IC3H7	6.46E + 12	874	1.16
618	C3H6 + H↔C3H5 + H2	3.25E + 11	4445	0
619	C3H6 + H↔SC3H5 + H2	1.95E + 12	4445	0
620	C3H6 + O2↔SC3H5 + HO2	1.95E + 12	39000	0
621	C3H6 + O2↔TC3H5 + HO2	1.95E + 12	39000	0
622	C3H6 + O2↔C3H5 + HO2	1.60E + 11	39000	0
623	C3H6 + CH3↔C3H5 + CH4	3.30E + 11	8800	0
624	C3H6 + CH3↔SC3H5 + CH4	5.00E + 10	10110	0
625	C3H6 + CH3↔TC3H5 + CH4	1.00E + 11	8030	0
626	C3H6 + C2H5↔C3H5 + C2H6	1.26E + 14	9800	0
627	C3H6O→C2H5 + HCO	3.16E + 11	58000	0
628	C3H5 + O2→CH2O + CH2O + CH	2.25E + 12	17210	0
629	C3H5 + HO2→C2H3 + CH2O + OH	3.33E + 12	0	0
630	C3H5 + H↔C3H4 + H2	1.81E + 14	0	0
631	C3H5 + O→C2H4 + CO + H	1.00E + 11	0	0
632	C3H5 + CH3↔C3H4 + CH4	4.00E + 11	0	0
633	C3H5 + C2H5↔C3H4 + C2H6	1.00E + 12	0	0
634	C3H5 + C2H3↔C3H4 + C2H4	4.34E + 12	0	0
635	SC3H5 + O2↔CH3HCO + HCO	4.50E + 12	0	0
636	SC3H5 + HO2→CH2CO + CH3 + OH	3.33E + 12	0	0
637	SC3H5 + H↔C3H4 + H2	1.81E + 14	0	0
638	SC3H5 + O→CH2CO + CH3	1.00E + 11	0	0
639	SC3H5 + CH3↔C3H4 + CH4	1.00E + 11	0	0
640	SC3H5 + C2H5↔C3H4 + C2H6	1.00E + 11	0	0
641	SC3H5 + C2H3↔C3H4 + C2H4	4.34E + 11	0	0
642	TC3H5 + O2↔CH3CO + CH2O	4.50E + 12	0	0
643	TC3H5 + HO2→CH2CO + CH3 + OH	3.33E + 12	0	0
644	TC3H5 + H↔C3H4 + H2	1.81E + 14	0	0
645	TC3H5 + O→HCCO + CH3 + H	1.00E + 11	0	0
646	TC3H5 + CH3↔C3H4 + CH4	1.00E + 11	0	0
647	TC3H5 + C2H5↔C3H4 + C2H6	1.00E + 11	0	0
648	TC3H5 + C2H3↔C3H4 + C2H4	2.00E + 18	0	0
649	C3H4 + M↔C3H3 + H + M	1.20E + 15	80000	0
650	C3H4↔PC3H4	4.00E + 13	92400	0
651	C3H4 + O2↔C3H3 + HO2	8.00E + 12	61500	0
652	C3H4 + HO2→CH2CO + CH2 + OH	3.12E + 12	19000	0
653	C3H4 + OH↔CH2CO + CH3	2.00E + 07	− 397	0
654	C3H4 + OH↔C3H3 + H2O	1.10E-02	1000	2
655	C3H4 + O↔C2H3 + HCO	2.00E + 12	− 4243	4.613
656	C3H4 + H↔C3H5	6.50E + 12	2700	0
657	C3H4 + H↔TC3H5	2.00E + 07	2000	0
658	C3H4 + H↔C3H3 + H2	2.00E + 11	5000	2
659	C3H4 + CH3↔C3H3 + CH4	4.70E + 18	7700	0
660	PC3H4 + M↔C3H3 + H + M	1.51E + 14	80000	0
661	C3H4CY↔C3H4	7.08E + 13	50400	0
662	C3H4CY↔PC3H4	2.00E + 08	43700	0
663	PC3H4 + O2→HCCO + OH + CH2	5.00E + 12	30100	1.5
664	PC3H4 + O2↔C3H3 + HO2	3.00E + 12	51000	0
665	PC3H4 + HO2→C2H4 + CO + OH	2.00E + 07	19000	0
666	PC3H4 + OH↔C3H3 + H2O	5.00E-04	1000	2
667	PC3H4 + OH↔CH2CO + CH3	6.40E + 12	− 1000	4.5
668	PC3H4 + O↔CH2CO + CH2	3.20E + 12	2010	0
669	PC3H4 + O↔C2H3 + HCO	6.30E + 12	2010	0
670	PC3H4 + O↔HCCO + CH3	3.20E + 11	2010	0
671	PC3H4 + O↔↔ > HCCO + CH2 + H	6.50E + 12	2010	0
672	PC3H4 + H↔TC3H5	2.00E + 07	2000	0
673	PC3H4 + H↔C3H3 + H2	1.30E + 05	5000	2
674	PC3H4 + H↔C2H2 + CH3	1.50E + 00	1000	2.5

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
675	PC3H4 + CH3↔C3H3 + CH4	1.00E + 12	5600	3.5
676	PC3H4 + C2H3↔C3H3 + C2H4	1.00E + 12	7700	0
677	PC3H4 + C3H5↔C3H3 + C3H6	5.00E + 13	7700	0
678	C3H3 + H→C3H2 + H2	1.39E + 14	3000	0
679	C3H3 + O→C2H + HCO + H	1.40E + 14	0	0
680	C3H3 + O→C2H2 + CO + H	1.00E + 13	0	0
681	C3H3 + OH→C3H2 + H2O	3.01E + 10	0	0
682	C3H3 + O2↔CH2CO + HCO	7.00E + 13	2870	0
683	C3H3 + CH↔IC4H3 + H	7.00E + 13	0	0
684	C3H3 + CH↔NC4H3 + H	4.00E + 13	0	0
685	C3H3 + CH2↔C4H4 + H	2.00E + 12	0	0
686	C3H3 + C3H3↔C6H5 + H	1.00E + 14	0	0
687	CH + C2H2→C3H2 + H	1.00E + 14	0	0
688	C3H2 + O2↔HCCO + CO + H	5.00E + 13	3000	0
689	C3H2 + OH↔C2H2 + HCO	3.00E + 13	0	0
690	C3H2 + CH2↔IC4H3 + H	4.11E + 18	0	0
691	C4H8↔IC4H7 + H	4.00E + 11	97350	−1
692	C4H8↔C2C4H8	4.00E + 11	60000	0
693	C4H8↔T2C4H8	8.00E + 16	60000	0
694	C4H8↔C3H5 + CH3	1.00E + 19	74000	0
695	C4H8↔C2H3 + C2H5	4.00E + 12	96770	−1
696	C4H8 + O2↔IC4H7 + HO2	1.00E + 11	33200	0
697	C4H8 + HO2↔IC4H7 + H2O2	6.50E + 12	17060	0
698	C4H8 + OH↔NC3H7 + CH2O	1.00E + 11	0	0
699	C4H8 + OH↔CH3HCO + C2H5	1.00E + 10	0	0
700	C4H8 + OH↔C2H6 + CH3CO	2.25E + 13	0	0
701	C4H8 + OH↔IC4H7 + H2O	2.51E + 12	2217	0
702	C4H8 + O↔C3H6 + CH2O	1.25E + 12	0	0
703	C4H8 + O↔CH3HCO + C2H4	1.63E + 13	850	0
704	C4H8 + O↔C2H5 + CH3CO	1.30E + 13	850	0
705	C4H8 + O↔IC4H7 + OH	1.80E + 05	4500	0
706	C4H8 + O↔NC3H7 + HCO	5.00E + 13	−1029	2.5
707	C4H8 + H↔IC4H7 + H2	1.00E + 11	3900	0
708	C4H8 + CH3↔IC4H7 + CH4	1.00E + 11	7300	0
709	C4H8 + C2H5↔IC4H7 + C2H6	7.90E + 10	8000	0
710	C4H8 + C3H5↔IC4H7 + C3H6	8.00E + 10	12400	0
711	C4H8 + SC3H5↔IC4H7 + C3H6	8.00E + 10	12400	0
712	C4H8 + TC3H5↔IC4H7 + C3H6	1.72E + 14	12400	0
713	C2C4H8↔T2C4H8	1.00E + 13	64280	0
714	C2C4H8↔C4H6 + H2	4.07E + 18	65500	0
715	C2C4H8↔IC4H7 + H	2.00E + 16	97350	−1
716	C2C4H8↔SC3H5 + CH3	1.25E + 14	95000	0
717	C2C4H8 + OH↔IC4H7 + H2O	1.40E + 13	3060	0
718	C2C4H8 + OH↔CH3HCO + C2H5	6.03E + 12	0	0
719	C2C4H8 + O↔IC3H7 + HCO	1.00E + 12	0	0
720	C2C4H8 + O↔CH3HCO + C2H4	1.00E + 13	0	0
721	C2C4H8 + H↔IC4H7 + H2	1.00E + 11	3500	0
722	C2C4H8 + CH3↔IC4H7 + CH4	4.07E + 18	8200	0
723	T2C4H8↔IC4H7 + H	2.00E + 16	97350	−1
724	T2C4H8↔SC3H5 + CH3	1.00E + 14	96000	0
725	T2C4H8 + OH↔IC4H7 + H2O	1.50E + 13	3060	0
726	T2C4H8 + OH↔CH3HCO + C2H5	6.03E + 12	0	0
727	T2C4H8 + O↔IC3H7 + HCO	1.00E + 12	0	0
728	T2C4H8 + O↔CH3HCO + C2H4	5.00E + 12	0	0
729	T2C4H8 + H↔IC4H7 + H2	1.00E + 11	3500	0
730	T2C4H8 + CH3↔IC4H7 + CH4	1.20E + 14	8200	0
731	IC4H7↔C4H6 + H	1.00E + 14	49300	0
732	IC4H7↔C2H4 + C2H3	3.16E + 12	49000	0
733	IC4H7 + H↔C4H6 + H2	1.00E + 11	0	0
734	IC4H7 + O2↔C4H6 + HO2	1.00E + 13	0	0
735	IC4H7 + CH3↔C4H6 + CH4	4.00E + 12	0	0
736	IC4H7 + C2H3↔C4H6 + C2H4	4.00E + 12	0	0
737	IC4H7 + C2H5↔C4H6 + C2H6	5.00E + 11	0	0
738	IC4H7 + C2H5↔C4H8 + C2H4	5.00E + 11	0	0
739	IC4H7 + C2H5↔T2C4H8 + C2H4	5.00E + 11	0	0
740	IC4H7 + C2H5↔C2C4H8 + C2H4	4.00E + 13	0	0
741	IC4H7 + C3H5↔C4H6 + C3H6	3.16E + 12	0	0
742	IC4H7 + IC4H7↔C4H6 + C4H8	3.00E + 12	0	0
743	C2H3 + C2H4↔C4H6 + H	3.00E + 07	1000	0
744	C4H6 + H↔NC4H5 + H2	3.00E + 07	13000	2
745	C4H6 + H↔IC4H5 + H2	2.00E + 07	6000	2
746	C4H6 + OH↔NC4H5 + H2O	2.00E + 07	5000	2
747	C4H6 + OH↔IC4H5 + H2O	1.00E + 12	2000	2
748	C4H6 + O↔C2H4 + CH2CO	1.00E + 12	0	0
749	C4H6 + O↔PC3H4 + CH2O	2800	0	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
750	C2H2 + NC4H5↔C6H6 + H	2.00E + 07	1400	2.9
751	NC4H5 + OH↔C4H4 + H2O	3.00E + 07	1000	2
752	NC4H5 + H↔C4H4 + H2	1.00E + 14	1000	2
753	NC4H5 + H↔IC4H5 + H	2.00E + 15	0	0
754	IC4H5↔C4H4 + H	1.60E + 14	45000	0
755	NC4H5↔C4H4 + H	1.00E + 07	41400	0
756	C4H4 + OH↔IC4H3 + H2O	7.50E + 06	2000	2
757	C4H4 + OH↔NC4H3 + H2O	2.00E + 07	5000	2
758	C4H4 + H↔NC4H3 + H2	1.00E + 14	15000	2
759	NC4H3 + H↔IC4H3 + H	2.00E + 13	0	0
760	IC4H3 + CH2↔C3H4 + C2H	1.00E + 12	0	0
761	IC4H3 + O2↔CH2CO + HCCO	3.00E + 13	0	0
762	IC4H3 + OH↔C4H2 + H2O	2.00E + 13	0	0
763	IC4H3 + O↔CH2CO + C2H	5.00E + 13	0	0
764	IC4H3 + H↔C4H2 + H2	2800	0	0
765	NC4H3 + C2H2↔C6H5	1.00E + 16	1400	2.9
766	NC4H3 + M↔C4H2 + H + M	4.46E + 15	59700	0
767	IC4H3 + M↔C4H2 + H + M	2.00E + 13	46516	0
768	IC4H3 + O↔H2C4O + H	5.00E + 13	0	0
769	H2C4O + H↔C2H2 + HCCO	1.00E + 07	3000	0
770	H2C4O + OH↔CH2CO + HCCO	6.66E + 12	2000	2
771	C4H2 + OH↔H2C4O + H	2.20E + 12	−410	0
772	C2H2 + C2H2↔IC4H3 + H	2.20E + 14	64060	0
773	C4H2 + M↔C4H + H	1.20E + 12	116740	0
774	C4H2 + O↔C3H2 + CO	1.82E + 14	0	0
775	C2H2 + C2H↔C4H2 + H	1.00E + 14	467	0
776	C4H + O2↔C2H + CO + CO	5.00E + 13	0	0
777	C2O + H↔CH + CO	5.00E + 13	0	0
778	C2O + O↔CO + CO	2.00E + 13	0	0
779	C2O + OH↔CO + CO + H	2.00E + 13	0	0
780	C2O + O2↔CO + CO + O	4.00E + 05	0	0
781	C2 + H2↔C2H + H	5.00E + 13	1000	2.4
782	C2 + O2↔CO + CO	5.00E + 13	0	0
783	C2 + OH↔C2O + H	5.00E + 13	0	0
784	C6H5 + OH↔C6H5O + H	2.10E + 12	0	0
785	C6H5 + O2↔C6H5O + O	5.00E + 13	7470	0
786	C6H5 + HO2↔C6H5O + OH	1.74E + 14	1000	0
787	C6H6 + H↔C6H5 + H2	1.68E + 08	10360	0
788	C6H6 + OH↔C6H5 + H2O	2.78E + 13	1450	1.42
789	C6H6 + O↔C6H5O + H	4.00E + 13	4910	0
790	C6H6 + O2↔C6H5O + OH	7.10E + 13	34000	0
791	H + C6H5↔C6H6	3.80E + 13	670	0
792	C3H3 + O→C2H3 + CO	2.00E + 13	0	0
793	C3H3 + O↔CH2O + C2H	6.00E + 12	0	0
794	C3H3 + O2→HCCO + CH2O	1.00E + 13	0	0
795	C3H3 + CH3↔C2H5 + C2H	5.00E + 12	37500	0
796	C3H3 + CH3↔C4H6	3.00E + 12	0	0
797	C3H6 + C2H3↔C3H5 + C2H4	1.30E + 11	14500	0
798	C3H6 + CH3O↔C3H5 + CH3OH	1.20E + 13	4000	0
799	CH2 + C2H2↔C3H4	5.00E + 14	6620	0
800	C3H4 + C3H4↔C3H5 + C3H3	1.70E + 12	64700	0
801	C3H4 + OH↔CH2O + C2H3	1.70E + 12	−300	0
802	C3H4 + OH↔HCO + C2H4	1.00E + 12	−300	0
803	C3H4 + O↔CH2O + C2H2	7.80E + 12	0	0
804	C3H4 + O→CO + C2H4	2.00E + 12	1600	0
805	C3H4 + C3H5↔C3H3 + C3H6	1.00E + 13	7700	0
806	C3H4 + C2H↔C3H3 + C2H2	4.20E + 16	0	0
807	PC3H4↔C2H + CH3	1.00E + 13	100000	0
808	PC3H4 + C2H↔C3H3 + C2H2	1.00E + 13	0	0
809	C3H2 + O2↔HCO + HCCO	2.51E + 05	0	0
810	C2H2 + C2H3↔NC4H5	4.00E + 13	2100	1.9
811	C2H3 + C2H3↔IC4H5 + H	3.00E + 07	0	0
812	IC4H5 + H↔C4H4 + H2	1.00E + 14	1000	2
813	C4H2 + H↔C4H + H2	7.23E + 12	35000	0
814	C4H6 + OH↔C3H5 + CH2O	3.98E + 10	−994	0
815	C4H8 + IC4H7↔IC4H7 + C2C4H8	3.98E + 10	12400	0
816	C4H8 + IC4H7↔IC4H7 + T2C4H8	3.00E + 11	12400	0
817	C3H3 + C3H3↔C6H6	1.40E + 12	0	0
818	C3H3 + C3H4→C6H6 + H	1.02E + 13	10000	0
819	C3H5 + C3H5↔C6H10	1.00E + 16	−263	0
820	C6H10→C6H9 + H	3.70E + 13	85000	0
821	C6H10 + OH→C6H9 + H2O	5.00E + 13	0	0
822	C6H9→C2H3 + C4H6	1.48E + 12	38000	0
823	C2H3 + C4H6→C6H9	1.25E + 12	3240	−0.17
824	C3H5 + C2H5↔C3H6 + C2H4	8.00E + 12	0	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
825	C3H6 + OH↔C2H5 + CH2O	3.40E + 11	0	0
826	C3H6 + OH↔CH3 + CH3HCO	6.00E + 11	0	0
827	C3H5 + O2↔C3H4 + HO2	8.00E + 10	10000	0
828	CH2O + C3H5↔HCO + C3H6	3.80E + 11	12400	0
829	CH3HCO + C3H5↔CH3CO + C3H6	6.03E + 12	7200	0
830	C3H8 + CH3O2↔NC3H7 + CH3O2H	1.99E + 12	19380	0
831	C3H8 + CH3O2↔IC3H7 + CH3O2H	6.03E + 12	17050	0
832	$C_3H_8 + C_2H_5O_2 \leftrightarrow NC_3H_7 + C_2H_5O_2H$	1.99E + 12	19380	0
833	$C_3H_8 + C_2H_5O_2 \leftrightarrow IC_3H_7 + C_2H_5O_2H$	6.03E + 12	17050	0
834	$C_3H_8 + IC_3H_7O_2 \leftrightarrow NC_3H_7 + IC_3H_7O_2H$	1.99E + 12	19380	0
835	$C_3H_8 + IC_3H_7O_2 \leftrightarrow IC_3H_7 + IC_3H_7O_2H$	6.03E + 12	17050	0
836	$C_3H_8 + NC_3H_7O_2 \leftrightarrow NC_3H_7 + NC_3H_7O_2H$	1.99E + 12	19380	0
837	$C_3H_8 + NC_3H_7O_2 \leftrightarrow IC_3H_7 + NC_3H_7O_2H$	4.82E + 12	17050	0
838	$NC_3H_7 + O_2 \leftrightarrow NC_3H_7O_2$	6.62E + 12	0	0
839	$IC_3H_7 + O_2 \leftrightarrow IC_3H_7O_2$	3.20E + 13	0	0
840	$NC_3H_7 + HO_2 \leftrightarrow NC_3H_7O + OH$	3.20E + 13	0	0
841	$IC_3H_7 + HO_2 \leftrightarrow IC_3H_7O + OH$	3.80E + 12	0	0
842	$NC_3H_7 + CH_3O_2 \leftrightarrow NC_3H_7O + CH_3O$	3.80E + 12	−1200	0
843	$IC_3H_7 + CH_3O_2 \leftrightarrow IC_3H_7O + CH_3O$	3.80E + 12	−1200	0
844	$NC_3H_7 + NC_3H_7O_2 \leftrightarrow NC_3H_7O + NC_3H_7O$	3.80E + 12	−1200	0
845	$IC_3H_7 + NC_3H_7O_2 \leftrightarrow IC_3H_7O + NC_3H_7O$	3.80E + 12	−1200	0
846	$NC_3H_7 + IC_3H_7O_2 \leftrightarrow NC_3H_7O + IC_3H_7O$	3.80E + 12	−1200	0
847	$IC_3H_7 + IC_3H_7O_2 \leftrightarrow IC_3H_7O + IC_3H_7O$	4.60E + 10	−1200	0
848	$NC_3H_7O_2 + HO_2 \leftrightarrow NC_3H_7O_2H + O_2$	4.60E + 10	−2600	0
849	$IC_3H_7O_2 + HO_2 \leftrightarrow IC_3H_7O_2H + O_2$	3.80E + 12	−2600	0
850	$CH_3 + NC_3H_7O_2 \leftrightarrow CH_3O + NC_3H_7O$	3.80E + 12	−1200	0
851	$CH_3 + IC_3H_7O_2 \leftrightarrow CH_3O + IC_3H_7O$	4.00E + 15	−1200	0
852	$NC_3H_7O_2H \leftrightarrow NC_3H_7O + OH$	4.00E + 15	43000	0
853	$IC_3H_7O_2H \leftrightarrow IC_3H_7O + OH$	5.00E + 13	43000	0
854	$NC_3H_7O \leftrightarrow C_3H_5 + CH_2O$	4.00E + 14	15700	0
855	$IC_3H_7O \leftrightarrow CH_3 + CH_3HCO$	2.79E + 12	17200	0
856	$C_3H_6 + OH \leftrightarrow C_3H_6OH$	1.40E + 09	−1040	0
857	$C_3H_6OH \rightarrow C_3H_5 + CH_2O$	1.00E + 09	17200	0
858	$C_3H_6OH \rightarrow CH_3 + CH_3HCO$	1.00E + 12	17200	0
859	$C_3H_6OH + O_2 \leftrightarrow O_2C_3H_6OH$	1.00E + 16	−1100	0
860	$O_2C_3H_6OH \rightarrow CH_3HCO + CH_2O + OH$	3.20E + 11	25000	0
861	$C_3H_6 + CH_3O_2 \leftrightarrow C_3H_5 + CH_3O_2H$	1.05E + 11	14900	0
862	$C_3H_6 + CH_3O_2 \leftrightarrow C_3H_6O + CH_3O$	3.20E + 11	14200	0
863	$C_3H_6 + C_2H_5O_2 \leftrightarrow C_3H_5 + C_2H_5O_2H$	3.20E + 11	14900	0
864	$C_3H_6 + C_3H_5O_2 \leftrightarrow C_3H_5 + C_3H_5O_2H$	1.05E + 11	14900	0
865	$C_3H_6 + C_3H_5O_2 \leftrightarrow C_3H_6O + C_3H_5O$	3.20E + 11	14200	0
866	$C_3H_6 + CH_3CO_3 \leftrightarrow C_3H_5 + CH_3CO_3H$	3.20E + 11	14900	0
867	$C_3H_6 + NC_3H_7O_2 \leftrightarrow C_3H_5 + NC_3H_7O_2H$	3.20E + 11	14900	0
868	$C_3H_6 + IC_3H_7O_2 \leftrightarrow C_3H_5 + IC_3H_7O_2H$	1.20E + 10	14900	0
869	$C_3H_5 + O2 \leftrightarrow C_3H_5O_2$	9.00E + 12	−2300	0
870	$C_3H_5 + HO_2 \leftrightarrow C_3H_5O + OH$	3.80E + 11	0	0
871	$C_3H_5 + CH_3O_2 \leftrightarrow C_3H_5O + CH_3O$	3.80E + 11	−1200	0
872	$C_3H_5O_2 + CH_3 \leftrightarrow C_3H_5O + CH_3O$	3.80E + 11	−1200	0
873	$C_3H_5O_2 + C_3H_5 \leftrightarrow C_3H_5O + C_3H_5O$	4.60E + 10	−1200	0
874	$C_3H_5O_2 + HO_2 \leftrightarrow C_3H_5O_2H + O_2$	1.00E + 12	−2600	0
875	$C_3H_5O_2 + HO_2 \rightarrow C_3H_5O + OH + O_2$	3.70E + 12	0	0
876	$C_3H_5O_2 + CH_3O_2 \rightarrow C_3H_5O + CH_3O + O_2$	3.70E + 12	2200	0
877	$C_3H_5O_2 + C_3H_5O_2 \rightarrow C_3H_5O + C_3H_5O + O_2$	1.00E + 14	2200	0
878	$C_3H_5O \leftrightarrow CH_2O + C_2H_3$	4.00E + 15	21600	0
879	$C_3H_5O_2H \leftrightarrow C_3H_5O + OH$	1.30E + 11	43000	0
880	$CH_2O + C_3H_5O_2 \leftrightarrow HCO + C_3H_5O_2H$	1.30E + 11	10500	0
881	$CH_2O + NC_3H_7O \leftrightarrow HCO + NC_3H_7O_2H$	1.30E + 11	9000	0
882	$CH_2O + IC_3H_7O_2 \leftrightarrow HCO + IC_3H_7O_2H$	7.10E + 11	9000	0
883	$C_2H_4 + NC_3H_7O_2 \leftrightarrow C_2H_3 + NC_3H_7O_2H$	7.10E + 11	25000	0
884	$C_2H_4 + IC_3H_7O_2 \leftrightarrow C_2H_3 + IC_3H_7O_2H$	1.14E + 13	25000	0
885	$CH_4 + C_3H_5O_2 \leftrightarrow CH_3 + C_3H_5O_2H$	1.14E + 13	20460	0
886	$CH_4 + NC_3H_7O_2 \leftrightarrow CH_3 + NC_3H_7O_2H$	1.14E + 13	20460	0
887	$CH_4 + IC_3H_7O_2 \leftrightarrow CH_3 + IC_3H_7O_2H$	6.30E + 12	20460	0
888	$CH_3OH + NC_3H_7O_2 \leftrightarrow CH_2OH + NC_3H_7O_2H$	6.30E + 12	19360	0
889	$CH_3OH + IC_3H_7O_2 \leftrightarrow CH_2OH + IC_3H_7O_2H$	1.15E + 11	19360	0
890	$CH_3HCO + C_3H_5O_2 \leftrightarrow CH_3CO + C_3H_5O_2H$	1.15E + 11	10000	0
891	$CH_3HCO + NC_3H_7O_2 \leftrightarrow CH_3CO + NC_3H_7O_2H$	1.15E + 11	10000	0
892	$CH_3HCO + IC_3H_7O_2 \leftrightarrow CH_3CO + IC_3H_7O_2H$	6.00E + 13	10000	0
893	$C_2H + NO \leftrightarrow HCN + CO$	3.47E + 12	570	0
894	$CH_2 + NO \leftrightarrow HCN + OH$	3.20E + 16	−376	0
895	$C_2N_2 + M \leftrightarrow CN + CN + M$	6.00E + 13	94400	0
896	$CN + N_2O \leftrightarrow CNN + NO$	1.80E + 10	15360	0
897	$CN + N_2O \leftrightarrow CNN + NO$	3.10E + 12	1450	0
898	$CH + N_2 + M \leftrightarrow HCNN$	5.00E + 13	0	0.15
899	$HCNN + H \leftrightarrow H_2 + CNN$	2.00E + 13	0	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
900	$HCNN + H \rightarrow CH_2 + N_2$	2.00E + 13	3000	0
901	$HCNN + O \leftrightarrow OH + CNN$	5.00E + 13	20000	0
902	$HCNN + O \leftrightarrow CO + H + N_2$	5.00E + 13	15000	0
903	$HCNN + O \leftrightarrow HCN + NO$	1.00E + 13	15000	0
904	$HCNN + OH \leftrightarrow H_2O + CNN$	1.00E + 13	8000	0
905	$HCNN + OH \leftrightarrow H + HCO + N_2$	1.00E + 12	16000	0
906	$HCNN + O_2 \leftrightarrow HO_2 + CNN$	1.00E + 13	4000	0
907	$CNN + O \leftrightarrow CO + N_2$	1.00E + 14	0	0
908	$CNN + O \leftrightarrow CN + NO$	1.00E + 13	20000	0
909	$CNN + OH \leftrightarrow H + CO + N_2$	5.00E + 14	1000	0
910	$CNN + H \leftrightarrow NH + CN$	1.00E + 12	40000	0
911	$CNN + OH \leftrightarrow HCN + NO$	5.00E + 13	1000	0
912	$CNN + H \leftrightarrow HCN + N$	1.00E + 13	25000	0
913	$CNN + O_2 \leftrightarrow NO + NCO$	1.20E + 13	5000	0
914	$CH_4 + NO_2 \leftrightarrow CH_3 + HONO$	1.50E + 13	30000	0
915	$CH_3 + NO_2 \leftrightarrow CH_3O + NO$	1.01E + 14	0	0
916	$CH + NO_2 \leftrightarrow HCO + NO$	5.90E + 13	0	0
917	$CH_2 + NO_2 \leftrightarrow CH_2O + NO$	1.00E + 11	0	0
918	$CN + NO \leftrightarrow N_2 + CO$	5.00E + 15	0	0
919	$HNCO + M \leftrightarrow H + NCO + M$	4.00E + 13	120000	0
920	$HNCO + N \leftrightarrow NH + NCO$	3.20E + 13	36000	0
921	$CH_3O + HNO \leftrightarrow CH_3OH + NO$	2.00E + 13	0	0
922	$NCO + HO_2 \leftrightarrow HNCO + O_2$	2.51E + 14	0	0
923	$N_2O + CO \leftrightarrow CO_2 + N_2$	1.00E + 12	46000	0
924	$N_2O + CH_2 \leftrightarrow CH_2O + N_2$	9.00E + 09	0	0
925	$N_2O + CH_3 \leftrightarrow CH_3O + N_2$	1.70E + 14	0	0
926	$N_2O + HCO \leftrightarrow CO_2 + H + N_2$	1.70E + 14	20000	0
927	$N_2O + HCCO \leftrightarrow CO + HCO + N_2$	6.59E + 16	25500	0
928	$N_2O + C_2H_2 \leftrightarrow HCCO + H + N_2$	1.00E + 11	61200	0
929	$N_2O + C_2H_3 \leftrightarrow CH_2HCO + N_2$	1.50E + 04	0	0
930	$HOCN + O \leftrightarrow NCO + OH$	2.00E + 07	4000	2.64
931	$HOCN + H \leftrightarrow NCO + H_2$	6.38E + 05	2000	2
932	$HOCN + OH \leftrightarrow NCO + H_2O$	4.93E + 14	2560	2
933	$CN + NO_2 \leftrightarrow CO + N_2O$	3.70E + 14	344	−0.752
934	$CN + NO_2 \leftrightarrow CO_2 + N_2$	3.67E + 06	344	−0.752
935	$CN + CO_2 \leftrightarrow NCO + CO$	1.50E + 13	26884	2.2
936	$HNCO + CN \leftrightarrow HCN + NCO$	1.80E + 13	0	0
937	$NCO + CN \leftrightarrow CNN + CO$	3.60E + 12	0	0
938	$HONO + NCO \leftrightarrow HNCO + NO_2$	6.00E + 12	0	0
939	$NCO + CH_2O \leftrightarrow HNCO + HCO$	3.68E + 07	0	0
940	$CH + N_2 \leftrightarrow HCN + N$	5.20E + 13	20723	1.42
941	$C + N_2 \leftrightarrow CN + N$	4.80E + 12	44700	0
942	$CH_2 + N_2 \leftrightarrow HCN + NH$	1.20E + 12	35850	0
943	$C_2 + N_2 \leftrightarrow CN + CN$	2.00E + 13	27600	0
944	$H_2CN + N \leftrightarrow N_2 + CH_2$	3.00E + 14	0	0
945	$H_2CN + M \leftrightarrow HCN + H + M$	2.00E + 13	22000	0
946	$C + NO \leftrightarrow CN + O$	4.00E + 13	0	0
947	$CH + NO \leftrightarrow HCN + O$	4.00E + 13	0	0
948	$CH + NO \leftrightarrow CN + OH$	4.00E + 13	0	0
949	$CH + NO \leftrightarrow CO + NH$	1.39E + 12	0	0
950	$CH_2 + NO \leftrightarrow HCNO + H$	1.66E + 12	−1100	0
951	$CH_3 + NO \leftrightarrow HCN + H_2O$	7.13E + 12	16040	0
952	$CH_3 + NO \leftrightarrow H_2CN + OH$	2.40E + 13	24040	0
953	$HCCO + NO \leftrightarrow HCNO + CO$	1.00E + 14	0	0
954	$SCH_2 + NO \leftrightarrow HCN + OH$	1.00E + 14	0	0
955	$HCNO + H \leftrightarrow HCN + OH$	5.00E + 13	12000	0
956	$CH_2 + N \leftrightarrow HCN + H$	1.30E + 13	0	0
957	$CH + N \leftrightarrow CN + H$	1.90E + 11	0	0
958	$N + CO_2 \leftrightarrow NO + CO$	5.00E + 13	3400	0
959	$N + HCCO \leftrightarrow HCN + CO$	7.10E + 13	0	0
960	$CH_3 + N \leftrightarrow H_2CN + H$	2.00E + 13	0	0
961	$C_2H_3 + N \leftrightarrow HCN + CH_2$	4.00E + 12	0	0
962	$CN + H_2O \leftrightarrow HCN + OH$	4.00E + 12	7400	0
963	$CN + H_2O \leftrightarrow HOCN + H$	5.85E + 04	7400	0
964	$OH + HCN \leftrightarrow HOCN + H$	1.70E + 11	12500	2.4
965	$OH + HCN \leftrightarrow HNCO + H$	6.44E + 10	8740	0
966	$OH + HCN \leftrightarrow NH_2 + CO$	1.00E + 13	11700	0
967	$HOCN + H \leftrightarrow HNCO + H$	1.38E + 04	0	0
968	$HCN + O \leftrightarrow NCO + H$	3450	4980	2.64
969	$HCN + O \leftrightarrow NH + CO$	2.70E + 09	4980	2.64
970	$HCN + O \leftrightarrow CN + OH$	2.00E + 04	26600	1.58
971	$CN + H2 \leftrightarrow HCN + H$	1.00E + 13	1600	2.87
972	$CN + O \leftrightarrow CO + N$	7.20E + 12	0	0
973	$CN + O_2 \leftrightarrow NCO + O$	6.00E + 13	−400	0
974	$CN + OH \leftrightarrow NCO + H$	1.51E + 07	0	0

(*continued on next page*)

Table. 1 (*continued*)

No.	Reaction	A	Ea (cal/mol)	N
975	$CN + HCN \leftrightarrow C_2N_2 + H$	5.32E+15	1530	1.71
976	$CN + NO_2 \leftrightarrow NCO + NO$	6.00E+12	344	−0.752
977	$CN + N_2O \leftrightarrow NCO + N_2$	4.57E+12	15360	0
978	$C_2N_2 + O \leftrightarrow NCO + CN$	1.86E+11	8880	0
979	$C_2N_2 + OH \leftrightarrow HNCO + CN$	5.50E+14	2900	0
980	$HNCO + H \leftrightarrow H_2 + NCO$	2.10E+14	27220	0
981	$HNCO + H \leftrightarrow NH_2 + CO$	1.10E+16	16890	0
982	$HNCO + M \leftrightarrow NH + CO + M$	2.20E+06	86000	0
983	$HNCO + O \leftrightarrow NCO + OH$	9.60E+07	11430	2.11
984	$HNCO + O \leftrightarrow NH + CO_2$	1.50E+08	8520	1.41
985	$HNCO + O \leftrightarrow HNO + CO$	3.45E+07	44012	1.57
986	$HNCO + OH \leftrightarrow NCO + H_2O$	3.00E+11	3600	1.5
987	$HNCO + HO_2 \leftrightarrow NCO + H_2O_2$	1.00E+12	29000	0
988	$HNCO + O_2 \leftrightarrow HNO + CO_2$	5.00E+12	35000	0
989	$HNCO + NH_2 \leftrightarrow NCO + NH_3$	3.00E+13	6200	0
990	$HNCO + NH \leftrightarrow NCO + NH_2$	1.10E+14	23700	0
991	$NCO + H \leftrightarrow NH + CO$	2.00E+13	2000	0
992	$NCO + O \leftrightarrow NO + CO$	2.00E+13	0	0
993	$NCO + N \leftrightarrow N_2 + CO$	5.00E+12	0	0
994	$NCO + OH \leftrightarrow NO + HCO$	2.20E+14	15000	0
995	$NCO + M \leftrightarrow N + CO + M$	4.60E+18	54050	0
996	$NCO + NO \leftrightarrow N_2O + CO$	5.80E+18	934	−2.01
997	$NCO + NO \leftrightarrow N_2 + CO_2$	2.00E+12	934	−2.01
998	$NCO + O_2 \leftrightarrow NO + CO_2$	3.60E+13	20000	0
999	$NCO + HCO \leftrightarrow HNCO + CO$	1.90E+14	0	0
1000	$NCO + NO_2 \leftrightarrow CO + NO + NO$	1.90E+14	−326	−0.646
1001	$NCO + NO_2 \leftrightarrow CO_2 + N_2O$	1.80E+13	−326	−0.646
1002	$NCO + HNO \leftrightarrow HNCO + NO$	1.80E+13	0	0
1003	$NCO + NCO \leftrightarrow CO + CO + N_2$	7.24E+13	0	0
1004	$NO + HCO \leftrightarrow CO + HNO$	9.00E+13	0	−0.4
1005	$NO_2 + CO \leftrightarrow CO_2 + NO$	8.40E+15	33800	0
1006	$NO_2 + HCO \leftrightarrow H + CO_2 + NO$	3.00E+12	1930	−0.75
1007	$CH_3O + NO_2 \leftrightarrow HONO + CH_2O$	4.40E+12	0	0
1008	$CH_3O + NO \leftrightarrow CH_2O + HNO$	1.00E+10	2050	0
1009	$NO_2 + CH_2O \leftrightarrow HONO + HCO$	3.00E+14	15100	0
1010	$NO + CH_2O \leftrightarrow HNO + HCO$	1.00E+13	42000	0
1011	$NO_2 + HCO \leftrightarrow HONO + CO$	1.00E+14	0	0
1012	$NO_2 + HCO \leftrightarrow OH + NO + CO$	2.70E+18	0	0
1013	$NCO + N \leftrightarrow NO + CN$	9.00E+04	17200	−0.995
1014	$CN + CH_4 \leftrightarrow HCN + CH_3$	2.80E+13	−300	2.64
1015	$C + NO \leftrightarrow CO + N$	1.00E+13	0	0
1016	$NH + CO_2 \leftrightarrow HNO + CO$	1.00E+13	14350	0
1017	$NCO + CH_4 \leftrightarrow HNCO + CH_3$	4.80E+12	8135	0
1018	$C + N_2O \leftrightarrow CN + NO$	3.00E+13	0	0
1019	$CH + NH_2 \leftrightarrow HCN + H + H$	5.00E+13	0	0
1020	$CH + NH \leftrightarrow HCN + H$	3.00E+13	0	0
1021	$CH_2 + NH \leftrightarrow HCN + H + H$	5.00E+13	0	0
1022	$CH_3 + N \leftrightarrow HCN + H + H$	1.00E+13	0	0
1023	$CH_4 + N \leftrightarrow NH + CH_3$	1.00E+13	24000	0
1024	$C_3H_3 + N \leftrightarrow HCN + C_2H_2$	1.34E+13	0	0
1025	$CH + N_2O \leftrightarrow HCN + NO$	1.34E+13	−510	0
1026	$CH + N_2O \leftrightarrow CO + H + N_2$	5.20E+12	−510	0

was described by a set of differential equations obtained from the detailed Konnov's hydrocarbon combustion mechanism and solved numerically by employing the Bader–Deuflhard algorithm (Bader and Deuflhard, 1983), corresponding to the kinetic parameters for all species involved in the proposed model as listed in Table 1. The starting integration time was set to 1.0×10^{-7} s due to the fast reaction. This value establishes the starting time step to integrate the Kintecus model. After the first integration, the value changed depending on the accuracy and stiffness of the model.

The pressure was assumed to be constant at 101.3 kPa throughout the simulation time with an initial temperature of 1500 K. By keeping the pressure constant, the volume will vary to keep the entire gaseous product at the constant pressure when the simulation started. Kintecus calculates the initial pressure by the equation below;

$$P_i = (n_1 + n_2 + n_3 + \ldots + n_i)\frac{RT}{V} \quad (2)$$

Where P_i is the initial pressure and n is the species concentration. Kintecus assumes that the initial volume as 1 L. It does not allow us to specify the value of the pressure of the system directly. The user must calculate and specify the initial concentration of the participating species using stoichiometric reaction equations so that the value of P_i = 1.0 atm = 101.3 kPa. The convergence of the system was set to $1.0 \times 10^{-5.}$

In this study, the concentration profiles for the free radicals, such as H, OH and O radical, and intermediates involve in the hydrogen-hydrocarbon combustion for various hydrogen compositions were numerically obtained using Kintecus code as it reached equilibrium.

The Kinetics simulations were carried out for 22 selected cases for

Table. 2
The conditions and compositions of the fuel mixtures.

Case No.	Mixtures	H_2 %	Hydro-carbon %	Concentration [mol/cm^3]			
				H_2	Hydro-carbon	O_2	N_2
1	Pure H_2	1	0	2.40E-06	0.00E+00	1.20E-06	4.52E-06
2	Pure CH_4	0	1	0.00E+00	7.72E-07	1.54E-06	5.80E-06
3	H_2-CH_4	0.2	0.8	1.79E-07	7.14E-07	1.52E-06	5.71E-06
4	H_2-CH_4	0.4	0.6	4.24E-07	6.36E-07	1.48E-06	5.58E-06
5	H_2-CH_4	0.6	0.4	7.81E-07	5.21E-07	1.43E-06	5.39E-06
6	H_2-CH_4	0.8	0.2	1.35E-06	3.38E-07	1.35E-06	5.08E-06
7	H_2-CH_4	0.9	0.1	1.79E-06	1.98E-07	1.29E-06	4.85E-06
8	H_2-CH_4	0.95	0.05	2.06E-06	1.09E-07	1.25E-06	4.70E-06
9	Pure C_2H_6	0	1	0.00E+00	4.60E-07	1.61E-06	3.05E-05
10	H_2-C_2H_6	0.2	0.8	1.10E-07	4.39E-07	1.59E-06	2.93E-05
11	H_2-C_2H_6	0.4	0.6	2.72E-07	4.08E-07	1.56E-06	2.76E-05
12	H_2-C_2H_6	0.6	0.4	5.36E-07	3.57E-07	1.52E-06	2.47E-05
13	H_2-C_2H_6	0.8	0.2	1.04E-06	2.60E-07	1.43E-06	1.93E-05
14	H_2-C_2H_6	0.9	0.1	1.52E-06	1.69E-07	1.35E-06	1.41E-05
15	H_2-C_2H_6	0.95	0.05	1.88E-06	9.92E-08	1.29E-06	1.01E-05
16	Pure C_3H_8	0	1	0.00E+00	3.27E-07	1.64E-06	6.16E-06
17	H_2-C_3H_8	0.2	0.8	7.92E-08	3.17E-07	1.62E-06	6.10E-06
18	H_2-C_3H_8	0.4	0.6	2.00E-07	3.00E-07	1.60E-06	6.02E-06
19	H_2-C_3H_8	0.6	0.4	4.08E-07	2.72E-07	1.56E-06	5.88E-06
20	H_2-C_3H_8	0.8	0.2	8.48E-07	2.12E-07	1.48E-06	5.58E-06
21	H_2-C_3H_8	0.9	0.1	1.32E-06	1.47E-07	1.40E-06	5.25E-06
22	H_2-C_3H_8	0.95	0.05	1.73E-06	9.12E-08	1.32E-06	4.97E-06

hydrogen-hydrocarbon mixtures at different compositions. Table 2 shows the fuel mixtures and compositions for each of the case.

3. Results and discussion

3.1. Free radicals

Figs. 1, 2 and 3 show the H, OH, and O maximum mole fraction profiles of H_2-CH_4, H_2-C_2H_6 and H_2-C_3H_8 flames at various hydrogen compositions. The reason that the authors have used maximum species mole fraction instead of species mole fraction at equilibrium as the main parameter is that because the concentration of O, OH and H radicals seem to be peaking at a certain time after simulation is initiated and then come down to the value observed at equilibrium (see Fig. 4). These results support the findings by Jeong and co-workers (Soo Kim et al., 2008) that the maximum mole fraction of these radicals at a certain time after combustion initiation process will always be higher compared to those at equilibrium condition for all hydrogen-methane mixtures. In this study, a similar trend can be observed in hydrogen-ethane and hydrogen-propane mixtures. Hence, the previous findings of Jeong and co-workers (Soo Kim et al., 2008) can be extended to both hydrogen-ethane and hydrogen-propane mixtures. This behaviour is due to the initiation of a chain reaction for H_2—O_2 system to form free radicals which cause the concentration of free radicals to peak and this is followed by slow three-body recombination reactions, hence a subtle drop of the concentration level of these radicals as it reached equilibrium.

As observed from Figs. 1, 2 and 3, the concentrations of H, OH and O radical increase upon the increase of hydrogen compositions for all hydrogen-hydrocarbon flames. The increment of the radical concentrations is crucial as the excess free radicals promote the combustion of the reactants by increasing the global reaction rate of the whole system, hence faster chemical kinetics.

The main reactions that grant the formation of H, OH and O are the H_2-O_2 initiation reactions (refer to Table 1 in Appendix 1 for a complete listing of the detailed Konnov's hydrocarbon oxidation mechanism) which are:

$$H_2 + O_2 \leftrightarrow OH + OH \quad \text{(R5)}$$

$$O + H_2 \leftrightarrow OH + H \quad \text{(R6)}$$

$$H + O_2 \leftrightarrow OH + O \quad \text{(R7)}$$

A significant increase in the production of OH, H and O radicals can be observed with the increase of H_2 ratio in the mixture. The reaction rate of R5 and R6 increase as hydrogen is added to the mixture hence forming more H and OH. Subsequently, the increase of H radical also increases the reaction rate of R7 to form more O and OH.

Figs. 1 and 2 also show that there is the small difference on the level of radical pool increments for hydrogen-methane, hydrogen-ethane and hydrogen-propane mixtures as hydrogen is added to the system. Higher mole fractions of OH and H radicals are observed for every increment of hydrogen in the hydrogen-methane flames followed by those in hydrogen-ethane and hydrogen-propane flames. It can be observed in Fig. 1 that in order for the H radical mole fraction in hydrogen-methane flame to increase 50% from the initial value, the hydrogen composition need to be increased to around 80%. The values are about 87% and 92% hydrogen addition for hydrogen-ethane and hydrogen-propane flame. A similar trend is also observed in Fig. 2 for OH maximum mole fraction. The increase in the concentration of OH and H mole fractions in the hydrogen-hydrocarbon mixtures is the main the reason for the increase of overall reaction rate via the chain branching reaction of R7.

Even though O radical maximum mole fraction in all hydrogen-hydrocarbon flames increases upon hydrogen addition, the significant increment at lower hydrogen addition can be observed for hydrogen-propane flame and descend in the order of hydrogen-ethane and hydrogen-methane flames (see Fig. 3). This is due to the fact that the O radical produced in R7 is used in R6 to produce more OH and H. Therefore, a higher concentration of OH and O radical pool in hydrogen-methane mixtures tend to consume more O radical to produce more OH and H radical compared to those in hydrogen-ethane and hydrogen-propane mixtures.

Since the overall reaction rate of a flame increases as the concentration of chain carrier radicals of O and OH, the results imply that at similar hydrogen compositions, the hydrogen-methane flame has higher reaction rate compare to hydrogen-ethane and hydrogen-propane flames. The plots also demonstrate that heavier hydrocarbon acts as a sink for the chain carrier radicals by consuming the radicals which support the findings by Wu et al. (Wu et al., 2007).

Moreover, the plots in Figs. 1 and 2 also show that significant increase of maximum H and OH mole fractions of hydrogen-methane flames can be observed at 40% hydrogen composition. However, the maximum H and OH mole fractions of hydrogen-ethane and hydrogen-propane flames only start to increase significantly at 60% and 80% H_2 compositions, respectively. Interestingly, similar trends can also be observed with the plot showing the burning velocity of hydrogen-hydrocarbon flames as a function of hydrogen compositions (see Fig. 5). This implies that there is a between the burning velocity of hydrogen-hydrocarbon flames and its maximum H and OH radical concentrations and this is further elaborated in Section 3

3.2. Emission indices

The measured CO and CO_2 mole fractions emitted by H_2-CH_4, H_2-C_2H_6 and H_2-C_3H_8 flames at various hydrogen compositions as calculated by Kintecus are shown in Figs. 6 and 7. As expected, CO and CO_2 emissions decrease as the hydrogen concentrations increase for all hydrogen-hydrocarbon flames.

The maximum CO mole fraction is around 0.049 for pure propane flame followed by 0.047 and 0.040 mole fractions for pure ethane and pure methane flame. A similar trend can also be observed for CO_2 production where pure propane flame produced the highest mole fraction of CO_2 at 0.061 mole fraction followed by those produced by pure ethane and pure methane flame at 0.058 and 0.051 mole fractions, respectively. On the other hand, the combustion of pure hydrogen does not produce CO since it does not have any C atom. The plots show that the amounts of CO and CO_2 produced by hydrogen-hydrocarbon flames decrease upon hydrogen addition. It also implies that the amount of CO_2 emitted from hydrogen-hydrocarbon combustion will always exceed the value of CO produced.

Referring to Konnov's hydrocarbon oxidation mechanism, the contributing reaction steps to CO production can be identified as R181 and R186 (see Table 1):

$$HCO + M \leftrightarrow H + CO + M \quad \text{(R181)}$$

$$HCO + O_2 \leftrightarrow CO + HO_2 \quad \text{(R186)}$$

However, a big portion of CO produced in the reactions is consumed by R178:

$$CO + OH \leftrightarrow CO_2 + H \quad \text{(R178)}$$

This is due to the fact that the activation energy for R178 is lower compares to R181 and R186, which means that R178 will react at higher rate compare to R181 and R186. Therefore, the amount of CO_2 produced will always exceed the value of CO for all hydrogen-hydrocarbon mixtures at all hydrogen compositions.

Moreover, it can be observed from the plots that different amount of H_2 compositions are needed by hydrogen-methane, hydrogen-ethane and hydrogen-propane flame in order to decrease the CO_2 production to half the amount produced by pure hydrocarbon. In order to significantly decrease the CO_2 production by hydrogen-methane flame, the hydrogen composition is needed to be increased up to 75% while the values are about 85% and 90% for hydrogen-ethane and hydrogen-propane. This signifies that hydrogen-hydrocarbon flames with a higher number of C atom need more hydrogen composition in order to decrease CO_2 emission at the same level as those produced by hydrogen-hydrocarbon flames with a lower number of C atom.

The results agree with the previous studies of Ilbas et al. (Ilbas et al., 2005), Jeong et al. (Soo Kim et al., 2008) and Burbano et al. (Burbano et al., 2008) where they have investigated the effects of hydrogen addition on hydrogen-methane on the CO emission and noticed that blending hydrogen with methane causes considerable reduction in CO and CO_2 emission. However, the data on hydrogen-ethane and hydrogen-propane mixtures are still lacking. This study has proved that similar characteristics also observed in these hydrogen-hydrocarbon mixtures, however, it must be noted that emission levels improvement as hydrogen is added to the system is more noticeable on hydrogen-methane flame compare to hydrogen-ethane and hydrogen-propane flame.

Fig. 8 shows the NO mole fraction profiles for H_2-CH_4, H_2-C_2H_6 and H_2-C_3H_8 flames as a function of hydrogen compositions. Contrary to those obtained for CO and CO_2 emissions, the addition of hydrogen in the hydrogen-hydrocarbon flames increases the NO emission levels. The behaviour can be observed for all hydrogen-hydrocarbon mixtures; however, the severity of the increment seems to increase in the trend of hydrogen-methane, hydrogen-ethane and hydrogen flames.

A significant increase of NO production in hydrogen-methane can be observed at around 80% hydrogen addition while hydrogen-ethane and hydrogen-propane flames display significant increase at 60% and 40% hydrogen addition. This indicates that at similar hydrogen content, NO production is substantially higher in hydrogen-propane flame compare to hydrogen-ethane and hydrogen-propane flames.

The reason for the increase of NO emission indices for hydrogen-hydrocarbon mixtures as hydrogen is added to the system is contributed by the increase of flame adiabatic temperature and also the concentration of H radical. According to Guo et al. (Guo et al., 2005), the most important NO formation is by the destruction of NO_2 by H radical. In Konnov mechanism, the reaction is represented by R104;

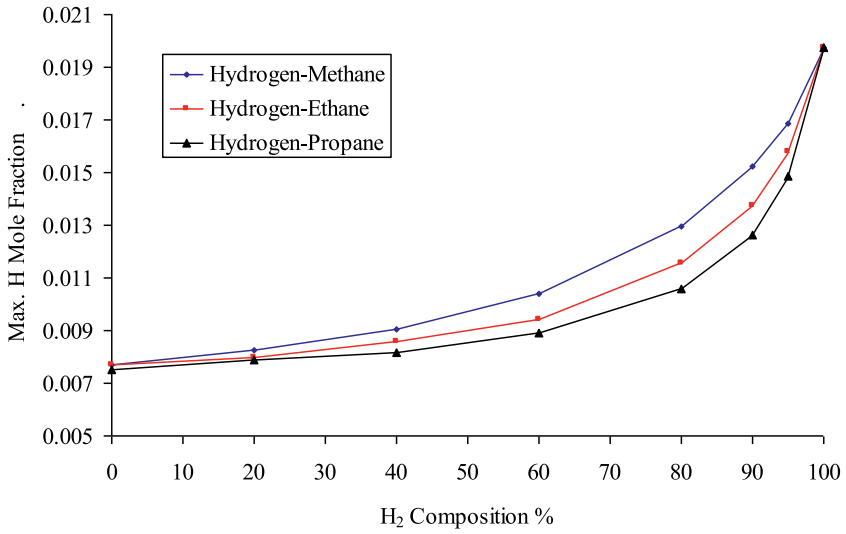

Fig. 1. Maximum H mole fraction profiles for H_2-CH_4, H_2-C_2H_6 and H_2-C_3H_8 flames as a function of H_2 compositions.

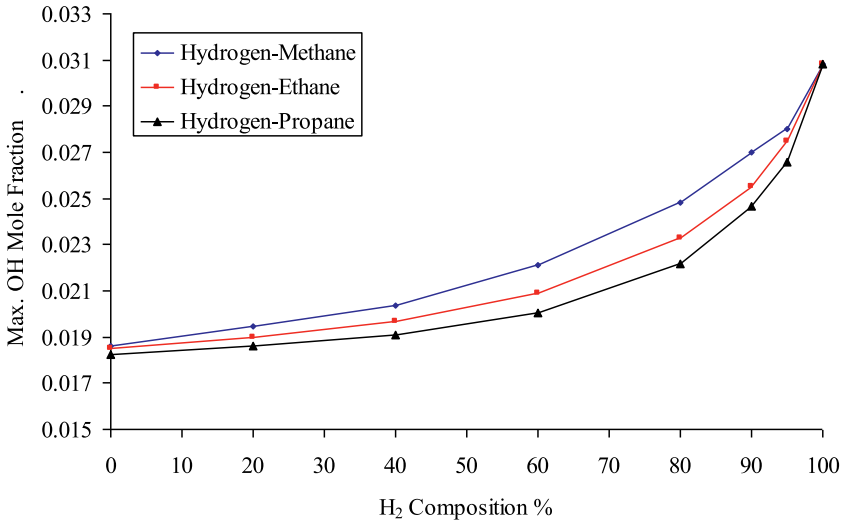

Fig. 2. Maximum OH mole fraction profiles for H_2-CH_4, H_2-C_2H_6 and H_2-C_3H_8 flames as a function of H_2 compositions.

$$NO_2 + H \leftrightarrow NO + OH \quad \text{(R104)}$$

The explanation of this behaviour is that the addition of hydrogen will increase the concentration of H and the combustion temperature (see next section). Subsequently, the reaction rate for R104 will also increase and more NO is formed. However, the reason behind the different level of NO production as hydrogen is added to hydrogen-methane, hydrogen-ethane and the hydrogen-propane flame are still unclear.

3.3. Adiabatic flame temperature

It is also known that the reaction rate coefficient in Arrhenius equation has a strong dependence on temperature. Therefore, it is suspected that temperature has a significant effect on chemical kinetics. It also directly affects the reactivity of the mixture since it also indicates the exothermicity and maximum temperature of the mixture. This statement signifies that a flame with higher reaction rate will produce higher temperature change compared to the flames with lower reaction rates. In this context, the temperature change is the difference between the temperature acquired when the mixture approaches equilibrium (i.e. adiabatic flame temperature T_{ad}) and the initial starting temperature T_o.

Fig. 9 shows the adiabatic flame temperature of the hydrogen-hydrocarbon mixtures calculated using Kintecus as functions of its H_2 composition at stoichiometric and equilibrium ($t = 5.0 \times 10^{-3}$ s) condition. It shows that for all hydrogen-hydrocarbon mixtures, the flame temperature increases with the increase of hydrogen content in the mixtures. However, hydrogen-methane flame shows the most significant increase of adiabatic flame temperature compared to hydrogen-ethane and hydrogen-propane flames. Initially, pure methane possesses the lowest flame temperature followed by pure ethane and pure propane. However, the flame temperature increases significantly as the hydrogen content in the mixtures becomes higher.

However, it is noted that the rate of flame temperature increase is much faster for hydrogen-methane flame compares to hydrogen-ethane and hydrogen-propane flames. At around 60% of hydrogen composition, the hydrogen-methane flame has the highest temperature at 3162 K followed by those of hydrogen-ethane and hydrogen-propane at 3157 K and 3151 K. This certainly shows that hydrogen addition has a significant impact on the temperature of hydrogen-methane mixtures

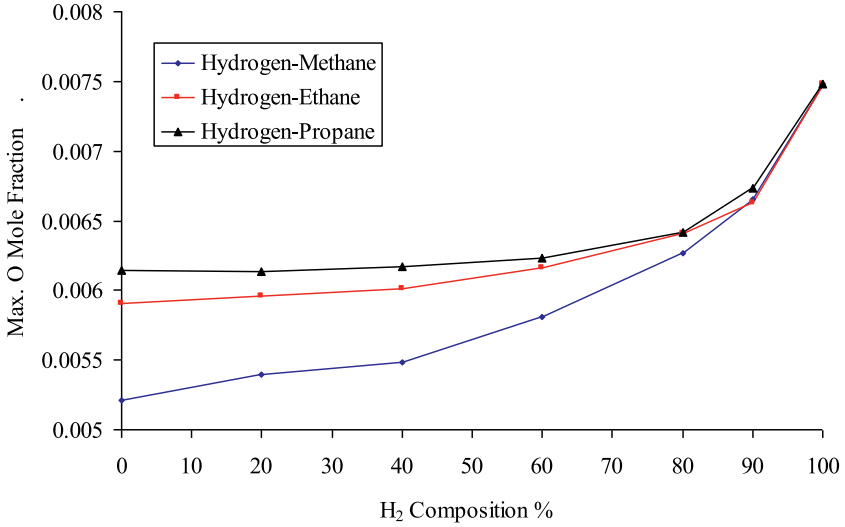

Fig. 3. Maximum O mole fraction profiles for H_2-CH_4, H_2-C_2H_6 and H_2-C_3H_8 flames as a function of H_2 compositions.

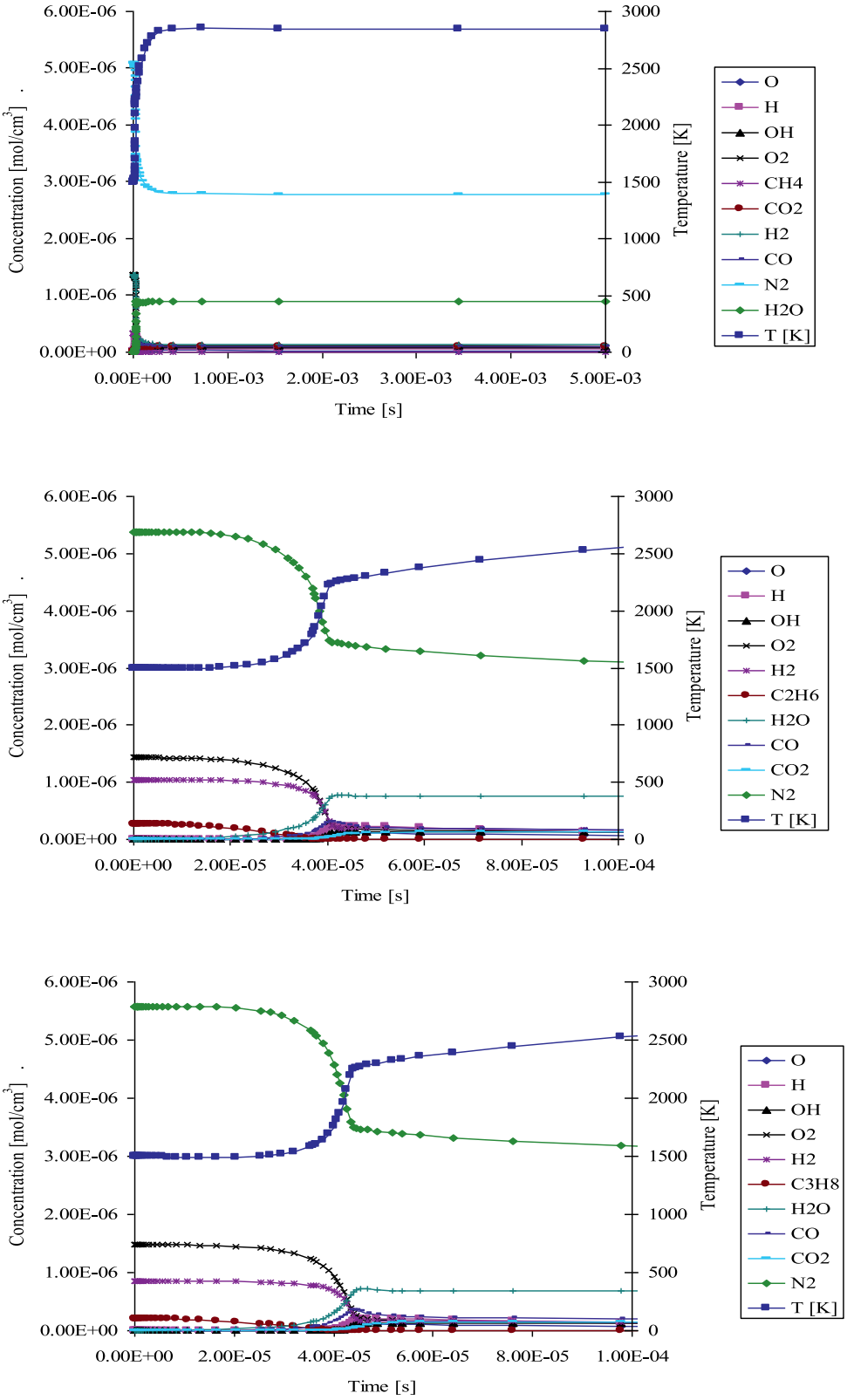

Fig. 4. Concentration profiles for 20% CH_4 80% H_2 (top), 20% C_2H_6 80% H_2 (middle), 20% C_3H_8 80% H_2 (bottom) at stoichiometric;

compared to other hydrogen-hydrocarbon mixtures studied. It can be observed from the plot that the hydrogen composition needs to be about 67% and 75% of for the hydrogen-ethane and hydrogen-propane mixtures to attain the same temperature of hydrogen-methane flame has 60% hydrogen composition.

The reasons for this behaviour are because of the higher energy input to the system and lower flame radiation upon hydrogen addition. The results have supported the theory made by Choudhuri and Gollahalli (2004) which have proposed that an increase in hydrogen content decreased the soot and carbon dioxide formation which denote

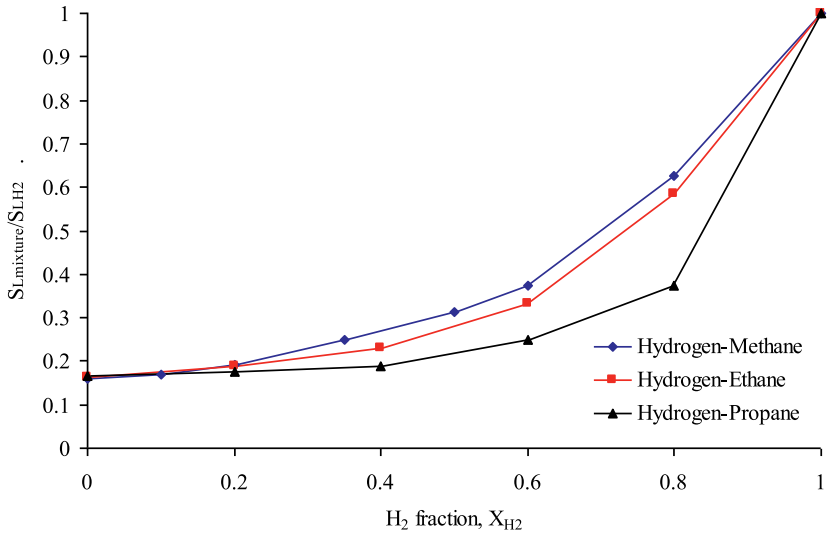

Fig. 5. The ratio of the laminar burning velocity of the hydrogen-hydrocarbon flames to the laminar burning velocity of pure hydrogen flame at the stoichiometric condition as a function of hydrogen concentrations.

the fact that radiative heat loss from the soot and carbon dioxide also decrease. In turn, the heat that is preserved by the system increases the temperature of the flame.

Since hydrogen-propane flame has the highest number of C atom compare to other lighter hydrogen-hydrocarbon flames, it tends to produce more soot and CO_2 (see the previous section). Therefore, more heat is lost through the combustion process, hence it lower flame temperature. Moreover, the temperature shift shown in Fig. 9 is attributed to the change of chemical kinetics of the hydrogen-hydrocarbon flames as hydrogen is added, with methane is more prone to be affected at smaller hydrogen addition compared to other heavier hydrocarbons. The effects of hydrogen addition on the chemical kinetics of hydrogen-hydrocarbon flames by influencing it free radical concentrations and the flame burning velocity will be discussed later in this chapter.

3.4. Laminar burning velocity

The laminar or fundamental flame velocity of hydrogen-air, hydrocarbon-air and hydrogen-hydrocarbon-air flames have been reported in several studies and the burning velocity values are presented in Fig. 5.

The measured laminar burning velocity of hydrogen flames in air peaked at a rich mixture of equivalence ratio 1.8 while the hydrogen-hydrocarbon-air flames assembled the features of hydrocarbon fuels, with the peak close to the stoichiometric. Comparing the magnitude of the burning velocity for the same equivalent ratio, the ascending order of the burning velocity for pure hydrocarbon fuels is methane, ethane and propane flames. However, the order is reversed as 50% of hydrogen is added to the system. This indicates that the hydrogen has a role in changing the chemical kinetics of hydrogen-hydrocarbon flames as shown in Fig. 5.

As seen from Figs. 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20 and 21, the increase of H and OH radicals in hydrogen-hydrocarbon flames upon hydrogen addition also increase the chain branching in the reaction zone of the flames through the reaction of $H + O_2 = OH + O$ chain branching reaction. Subsequently, the increment in chain branching and radical productions also increases the flame speed and thus the flammability of the hydrogen mixture. It is observed that strong correlation can be made between the mole fraction of (O + OH)

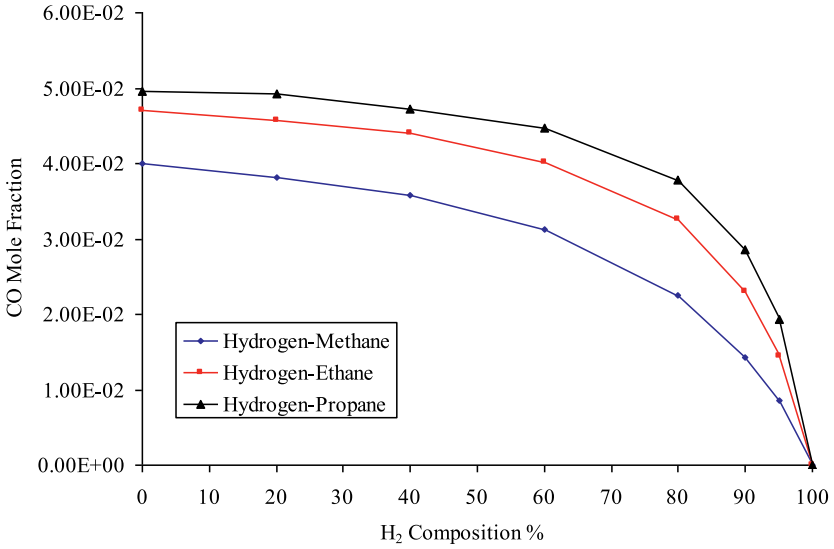

Fig. 6. CO mole fraction profiles for H_2-CH_4, H_2-C_2H_6 and H_2-C_3H_8 flames as a function of H_2 compositions.

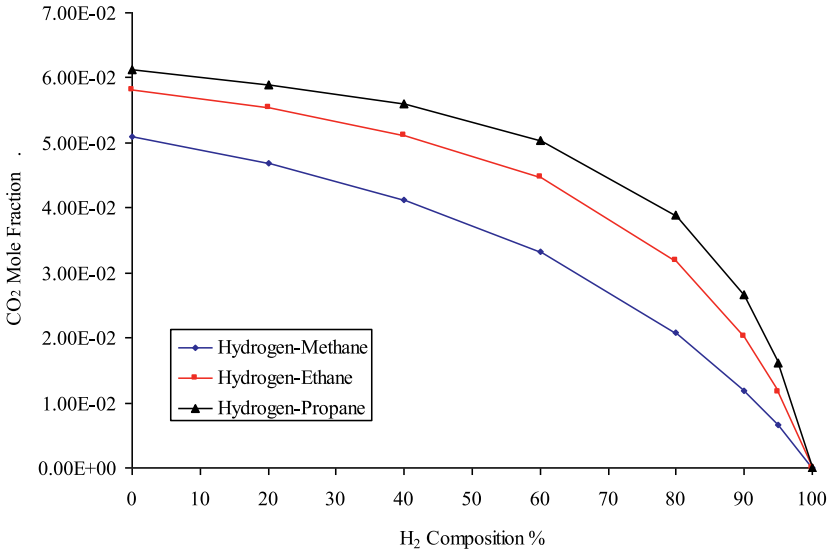

Fig. 7. CO_2 mole fraction profiles for H_2-CH_4, H_2-C_2H_6 and H_2-C_3H_8 flames as a function of H_2 compositions.

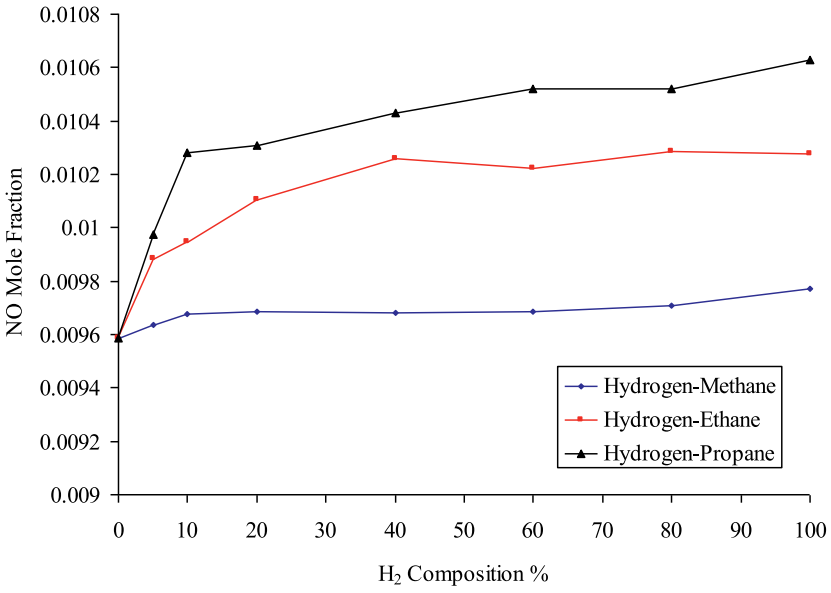

Fig. 8. NO mole fraction profiles for H_2-CH_4, H_2-C_2H_6 and H_2-C_3H_8 flames as a function of H_2 compositions.

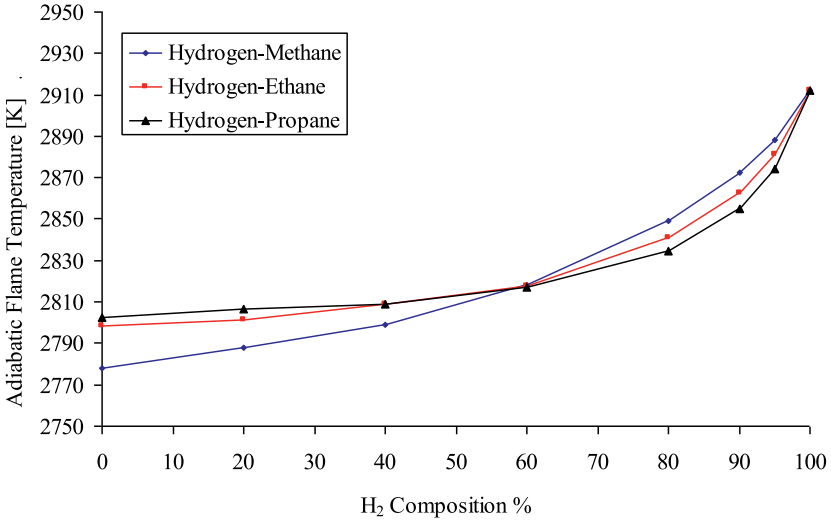

Fig. 9. Adiabatic flame temperature profiles of H_2-CH_4, H_2-C_2H_6 and H_2-C_3H_8 flames at equilibrium ($t = 5.0 \times 10^{-3}$ s) as a function of H_2 compositions.

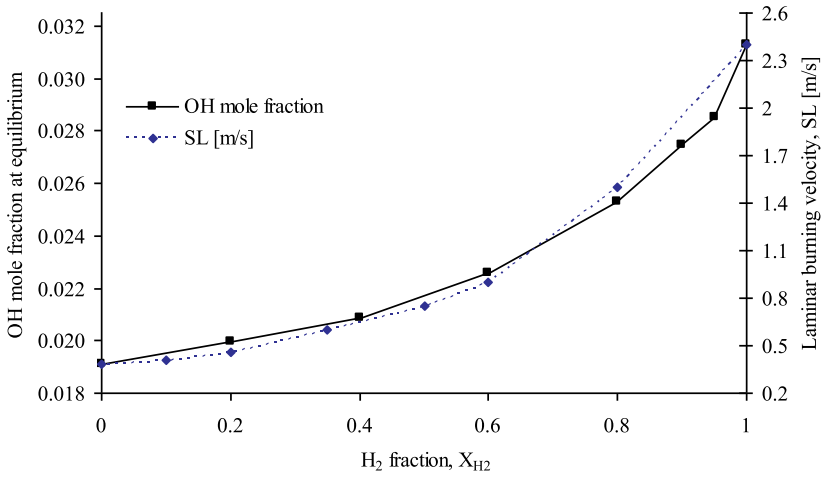

Fig. 10. Comparison between OH mole fraction and laminar burning velocity for hydrogen-methane flames at different hydrogen fractions.

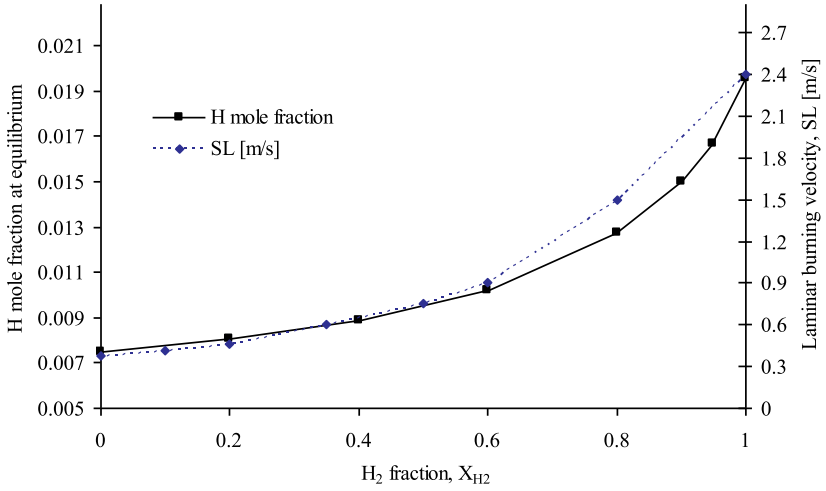

Fig. 11. Comparison between H mole fraction and laminar burning velocity for hydrogen-methane flames at different hydrogen fractions.

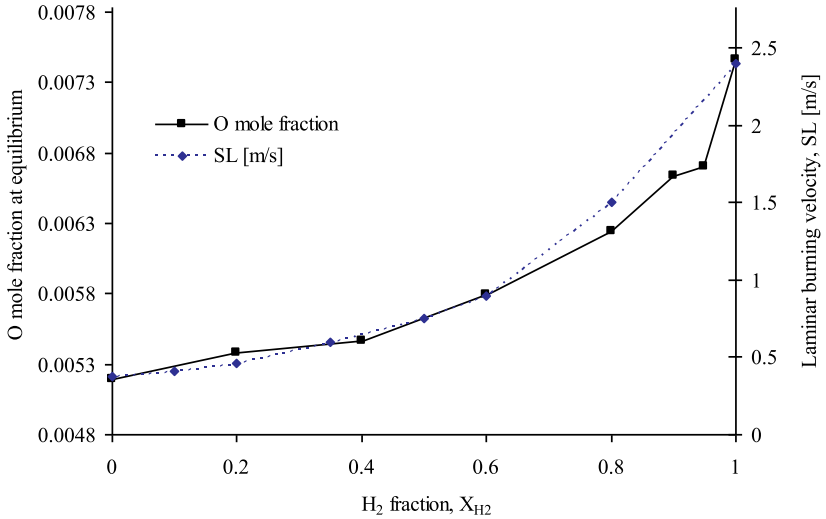

Fig. 12. Comparison between O mole fraction and laminar burning velocity for hydrogen-methane flames at different hydrogen fractions.

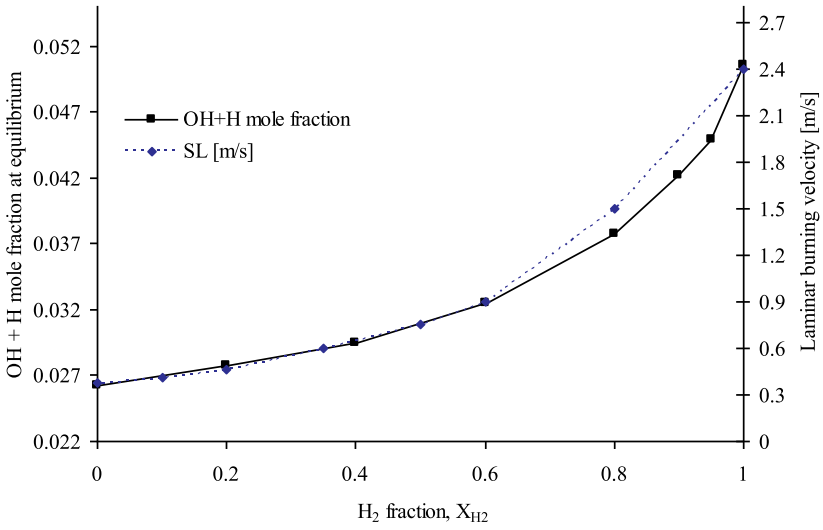

Fig. 13. Comparison between (OH + H) mole fraction and laminar burning hydrogen-methane flames mixtures at different hydrogen fractions.

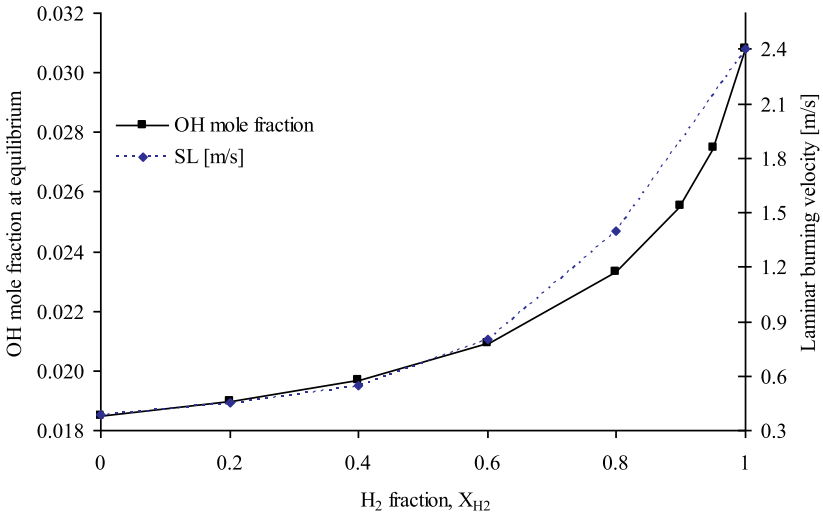

Fig. 14. Comparison between OH mole fraction and laminar burning velocity for hydrogen-ethane flames at different hydrogen fractions.

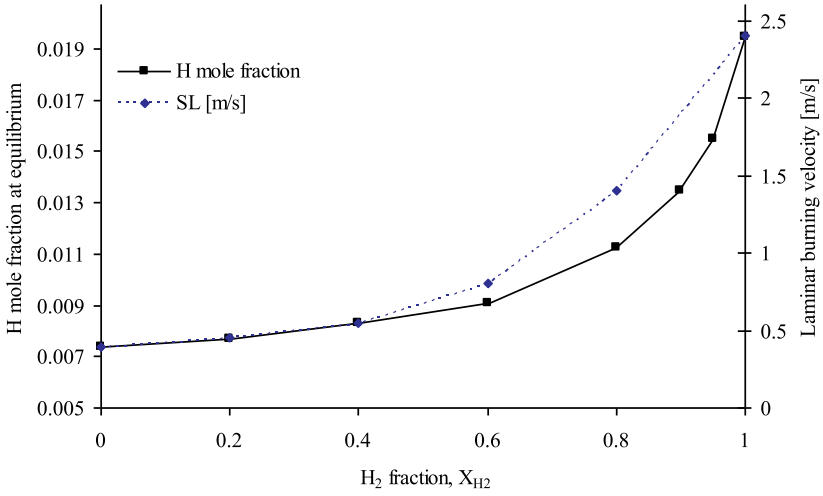

Fig. 15. Comparison between H mole fraction and laminar burning velocity for hydrogen-ethane flames at different hydrogen fractions.

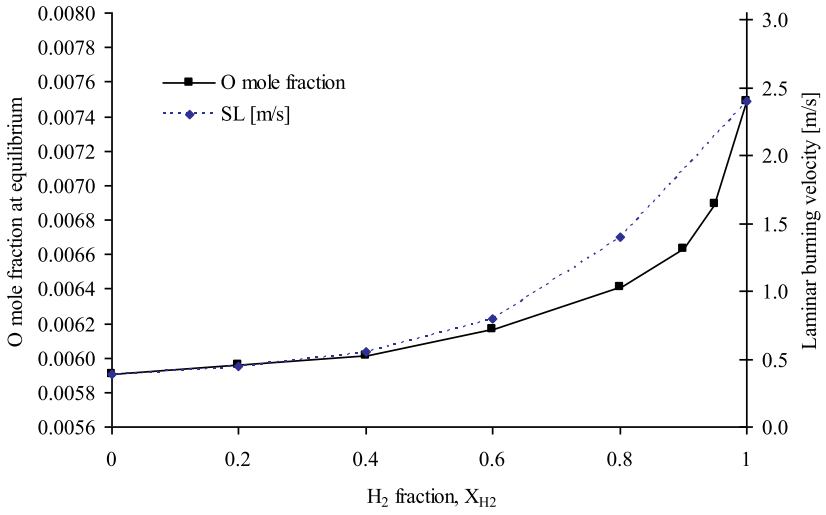

Fig. 16. Comparison between O mole fraction and laminar burning velocity for hydrogen-ethane flames at different hydrogen fractions.

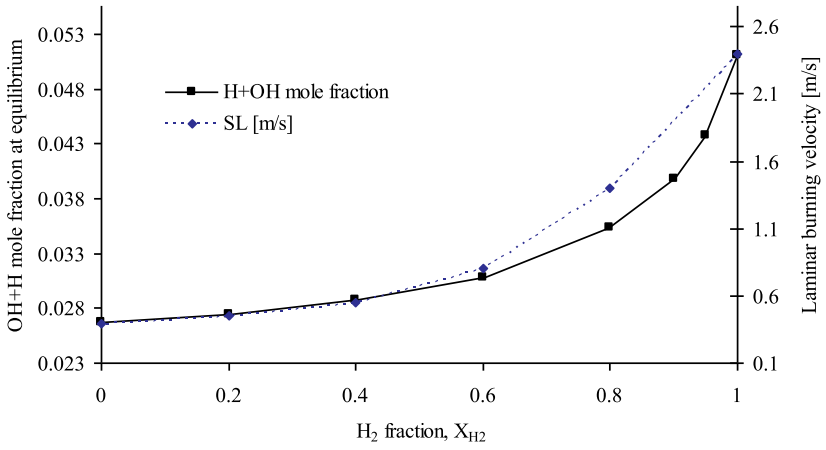

Fig. 17. Comparison between (OH + H) mole fraction and laminar burning hydrogen-ethane flames at different hydrogen fractions.

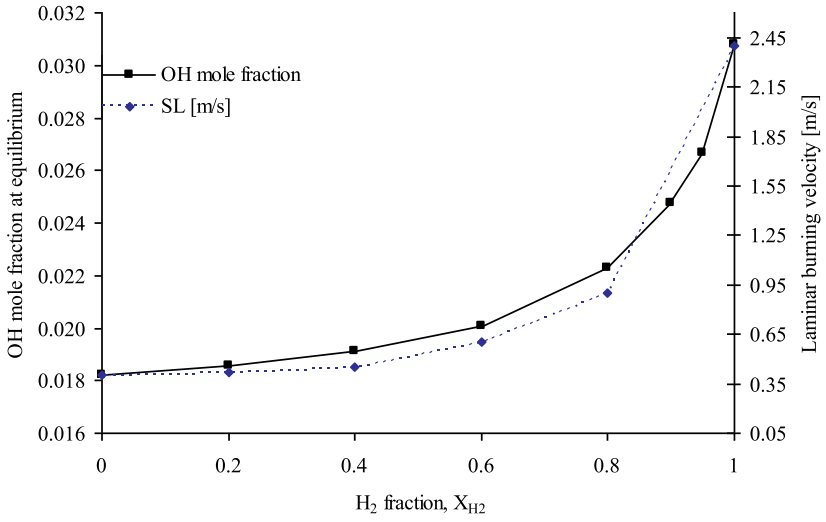

Fig. 18. Comparison between OH mole fraction and laminar burning velocity for hydrogen-propane flames at different hydrogen fractions.

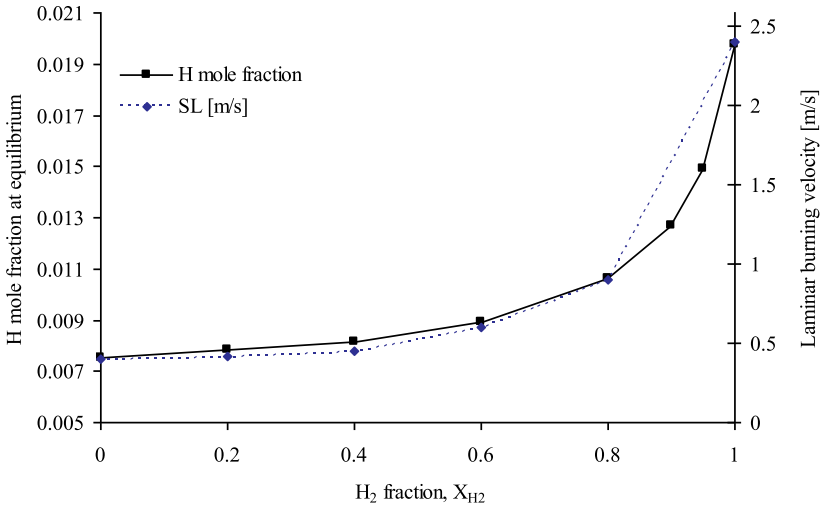

Fig. 19. Comparison between H mole fraction and laminar burning velocity for hydrogen-propane flames at different hydrogen fractions.

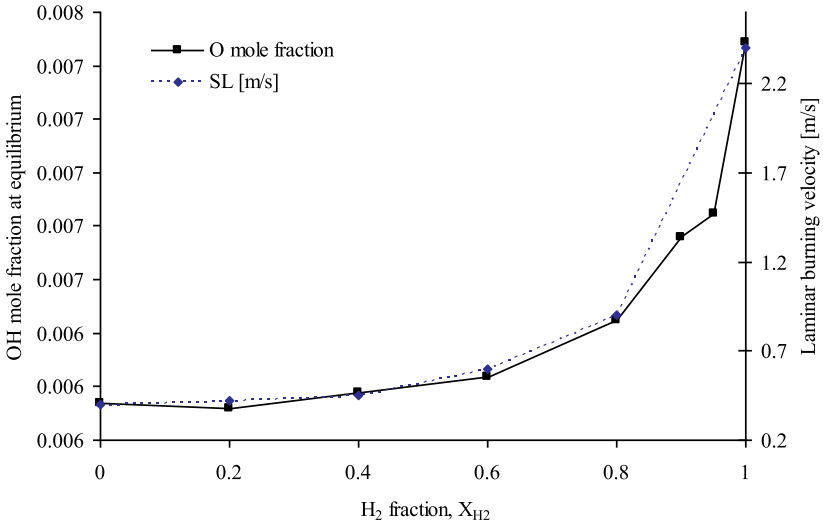

Fig. 20. Comparison between OH mole fraction and laminar burning velocity for hydrogen-propane flames at different hydrogen fractions.

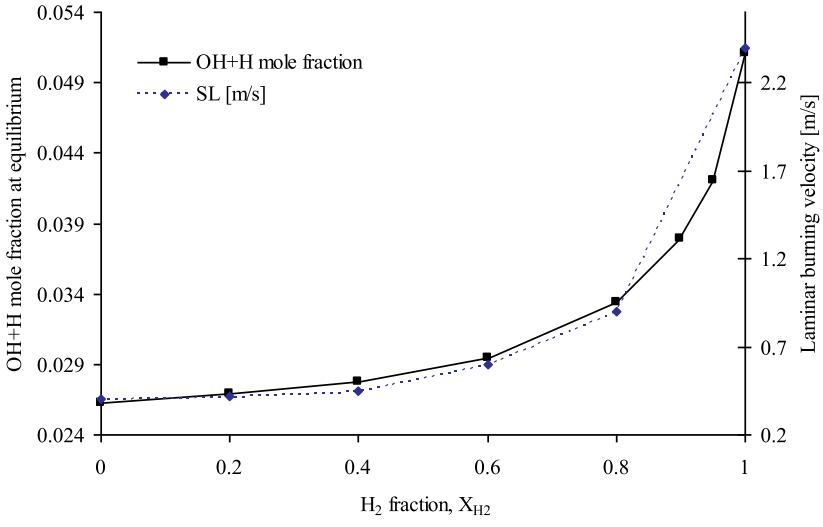

Fig. 21. Comparison between (OH + H) mole fraction and laminar burning velocity for hydrogen-propane flames at different hydrogen fractions.

radicals and the flame burning velocity even without the considering O mole fraction.

Even though the O radical mole fractions increase as hydrogen is added to the hydrogen-hydrocarbon flames, the value is not substantially high enough to influence the value of flame burning velocity. The value is about 10^{-1} lower than the mole fraction of OH and O radical.

4. Conclusions

Based on our study it was found that:

The concentration of free radicals O, OH and H increases as the hydrogen composition in the hydrogen-hydrocarbon flames increases. However, the hydrogen-methane mixture tends to be more affected by hydrogen addition compared to other mixtures. Hydrogen-propane mixture is the least affected mixture and it free radical concentrations will only increase rapidly if the hydrogen concentration is more than 80%.

- The combustion kinetics of hydrogen-hydrocarbon flame increase upon hydrogen addition. This is due to the increase of free radical pool concentrations and hence the flame global reaction rate.
- CO and CO_2 emissions decrease as the hydrogen concentration increase for all fuel mixtures. However, due to higher combustion temperature, a significant increase of NO production can be observed for all hydrogen-hydrocarbon mixtures.
- Hydrogen addition increases the adiabatic flame temperature of hydrogen-hydrocarbon mixtures. However, a very significant increase can be seen in methane-hydrogen mixture compared to other hydrogen-hydrocarbon mixtures.
- The strong correlation between the mole fractions of OH and H radical for hydrogen-methane, hydrogen-ethane and hydrogen-propane flames upon hydrogen addition to the system with the flame burning velocity.
- The extension of flame stability limits as hydrogen is added to hydrogen-hydrocarbon jet flames is due to the increasing free radical concentrations.

CRediT authorship contribution statement

Zine labidine Messaoudani: Writing - original draft, Writing - review & editing, Investigation, Formal analysis, Methodology, Validation, Visualization. **Mahar Diana Hamid:** Resources, Investigation, Writing - original draft, Supervision, Conceptualization, Project administration. **Che Rosmani Che Hassan:** Supervision, Conceptualization. **Yajue WU:** Supervision, Resources, Conceptualization, Project administration.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The authors would like to express the gratefulness and appreciation to FRGS Grant (Project No: RF012A-2018) from University of Malaya (UM).

Appendix 1

Appendix 2: Konnov's hydrocarbon combustion mechanism up to C3

References

Messaoudani, Z.l., Rigas, F, Binti Hamid, M.D, Che Hassan, C.R, 2016. Hazards, safety and knowledge gaps on hydrogen transmission via natural gas grid: a critical review. Int. J. Hydrogen Energy 41 (39), 17511–17525.
Rigas, F., Amyotte, P., 2012. Hydrogen Safety. CRC Press.
Rigas, F., Amyotte, P., 2013. Myths and facts about hydrogen hazards. 13th International Symposium on Loss Prevention and Safety Promotion in the Process Industries. Florence, Italy May 12-15, 2013).
Von Elbe, G., Lewis, B., 1948. The mechanism of the combustion of hydrocarbons. Proc. Symposium Combust. 1–2, 169–174.
Stone, R., Clarke, A., Beckwith, P., 1998. Correlations for the Laminar-Burning Velocity of Methane/Diluent/Air Mixtures Obtained in Free-Fall Experiments. Combust. Flame 114 (3–4), 546–555.
Daly, C.A., Simmie, J.M., Würmel, J., Djebaïli, N., Paillard, C., 2001. Burning velocities of dimethyl ether and air. Combust. Flame 125 (4), 1329–1340.
Ilbas, M., Crayford, A.P., Yilmaz, I., Bowen, P.J., Syred, N., 2006. Laminar-burning velocities of hydrogen-air and hydrogen-methane-air mixtures: An experimental study. Int. J. Hydrogen Energy 31 (12), 1768–1779.
Liao, S.Y., Jiang, D.M., Huang, Z.H., Shen, W.D., Yuan, C., Cheng, Q., 2007. Laminar burning velocities for mixtures of methanol and air at elevated temperatures. Energy Convers. Manag. 48 (3), 857–863.
Bradley, D., Lawes, M., Liu, K., Verhelst, S., Woolley, R., 2007. Laminar burning velocities of lean hydrogen-air mixtures at pressures up to 1.0 MPa. Combust. Flame 149 (1–2), 162–172.
Reyes, M., Tinaut, F.V., Horrillo, A., Lafuente, A., 2018. Experimental characterization of burning velocities of premixed methane-air and hydrogen-air mixtures in a constant volume combustion bomb at moderate pressure and temperature. Appl. Therm. Eng. 130, 684–697.
Hinton, N., Stone, R., Cracknell, R., Olm, C., 2018. Aqueous ethanol laminar burning velocity measurements using constant volume bomb methods. Fuel 214, 127–134.
Faghih, M., Chen, Z., 2016. The constant-volume propagating spherical flame method for laminar flame speed measurement. Sci. Bull. 61 (16), 1296–1310.
Lamoureux, N., Djebaïli-Chaumeix, N., Paillard, C.E., 2003. Laminar flame velocity determination for H2–air–He–CO2 mixtures using the spherical bomb method. Exp. Therm. Fluid Sci. 27 (4), 385–393.
Nair, M.R.S., Gupta, M.C., 1974. Burning velocity measurement by bomb method. Combust. Flame 22 (2), 219–221.
Lipatnikov, A.N., Shy, S.S., Li, W.-Y, 2015. Experimental assessment of various methods of determination of laminar flame speed in experiments with expanding spherical flames with positive Markstein lengths. Combust. Flame 162 (7), 2840–2854.
Reyes, M. and F.V. Tinaut. Characterization of the burning velocity of hydrogen/methane blends in a constant volume combustion bomb. in 2017 8th International Conference on Mechanical and Aerospace Engineering (ICMAE). 2017.
Yumlu, V.S., 1967. Prediction of burning velocities of carbon monoxide-hydrogen-air flames. Combust. Flame 11 (3), 190–194.
Sher, E., Ozdor, N., 1992. Laminar burning velocities of n-butane/air mixtures enriched with hydrogen. Combust. Flame 89 (2), 214–220.
El-Sherif, A.S., 1998. Effects of natural gas composition on the nitrogen oxide, flame structure and burning velocity under laminar premixed flame conditions. Fuel 77 (14), 1539–1547.
Turkeli-Ramadan, Z., Sharma, R.N., Raine, R.R., 2017. Experimental Study on Flat Flame Combustion for Ultra Micro Gas Turbine Applications. Combust. Sci. Technol. 189 (8), 1307–1325.
Günther, R., Janisch, G., 1972. Measurements of burning velocity in a flat flame front. Combust. Flame 19 (1), 49–53.
Gillespie, F., Metcalfe, W.K., Dirrenberger, P., Herbinet, O., Glaude, P.-A., Battin-Leclerc, F., Curran, H.J., 2012. Measurements of flat-flame velocities of diethyl ether in air. Energy 43 (1), 140–145.
Pang, Y., Li, Q., 2016. A review on kinetic models and corresponding analysis methods for hydrogen storage materials. Int. J. Hydrogen Energy 41 (40), 18072–18087.
Luo, M., Liu, D., 2017. Kinetic analysis of ethanol and dimethyl ether flames with hydrogen addition. Int. J. Hydrogen Energy 42 (6), 3813–3823.
Liu, D., 2014. Kinetic analysis of the chemical effects of hydrogen addition on dimethyl ether flames. Int. J. Hydrogen Energy 39 (24), 13014–13019.
Zhou, X., Jiang, X., Mira Martinez, D., 2016. The effects of chemical kinetic mechanisms on large eddy simulation (LES) of a nonpremixed hydrogen jet flame. Int. J. Hydrogen Energy 41 (26), 11427–11440.
Korsakova, A.I., Gubernov, V.V., Kolobov, A.V., Bykov, V., Maas, U., 2016. Stability of rich laminar hydrogen-air flames in a model with detailed transport and kinetic mechanisms. Combust. Flame 163, 478–486.
Luo, M., Liu, D., 2016. Combustion characteristics of primary reference fuels with

hydrogen addition. Int. J. Hydrogen Energy 41 (26), 11471–11480.
de Ferrières, S., El Bakali, A., Gasnot, L., Montero, M., Pauwels, J.F., 2013. Kinetic effect of hydrogen addition on natural gas premixed flames. Fuel 106, 88–97.
Hu, E., Huang, Z., He, J., Jin, C., Zheng, J., 2009. Experimental and numerical study on laminar burning characteristics of premixed methane-hydrogen-air flames. Int. J. Hydrogen Energy 34 (11), 4876–4888.
Fairweather, M., Ormsby, M.P., Sheppard, C.G.W., Woolley, R., 2009. Turbulent burning rates of methane and methane-hydrogen mixtures. Combust. Flame 156 (4), 780–790.
Wang, J., Huang, Z., Tang, C., Miao, H., Wang, X., 2009. Numerical study of the effect of hydrogen addition on methane-air mixtures combustion. Int. J. Hydrogen Energy 34 (2), 1084–1096.
Hu, E., Huang, Z., He, J., Miao, H., 2009. Experimental and numerical study on lean premixed methane-hydrogen-air flames at elevated pressures and temperatures. Int. J. Hydrogen Energy 34 (16), 6951–6960.
Glassman, I., 2008. Combustion. 4th ed. Academic Press Inc, LondonLondon Ltd.
Choudhuri, A.R.A.R., Gollahalli, S.R., 2004. Intermediate radical concentrations in hydrogen-natural gas blended fuel jet flames. Int. J. Hydrogen Energy 29 (12), 1293–1302.
Warnatz, J., 1985. Chemistry of high temperature combustion of alkanes up to octane. Symp. (Int.) Combust. 20 (1), 845–856.
Hughes, K.J., Tura´nyi, T., Clague, A.R., Pilling, M.J., 2001. Development and Testing of a Comprehensive Chemical Mechanism for the Oxidation of Methane. Int. J. Chem. Kinet. 33, 513–538.
Konnov, A., 2000. Development and validation of a detailed reaction mechanism for the combustion of small hydrocarbons. 28-th Symposium (Int.) on Combustion. Edinburgh, pp. 317.
Smith, G.P., G. D.M., M. Frenklach, N. Moriarty, B. Eiteneer, M. Goldenberg, C.T. Bowman, T.K. Hanson, S. Song, W.C. Gardiner, V.V. Lissianski, and Z. Qin. 2000; Available from: http://www.me.berkeley.edu/gri_mech/.
Hannebauer, B., Menzel, F., 2003. The Combustion of $SiCl_4$ in Hot O_2/H_2 Flames Z. Anorg. Allg. Chem. 629, 1485–1490.
Park, J., Jongsma, C.G., Zhang, R., North, S.W., 2004. OH/OD Initiated Oxidation of Isoprene in the Presence of O_2 and NO. J. Phys. Chem. A. 108, 10688–10697.
Shafir, E.V., Slagle, I.R., Knyazev, V.D., 2003. Kinetics and Products of the Self-Reaction of Propargyl Radicals. J. Phys. Chem. A 107 8893–8890.
Ianni, J.C., Bathe, K.J., 2003. A comparison of the Bader-Deuflhard and the Cash-Karp Runge-Kutta integrators for the GRI-MECH 3.0 model based on the chemical kinetics code Kintecus. Computational Fluid and Solid Mechanics 2003. Elsevier Science Ltd, Oxford, pp. 1368–1372.
Bader, G., Deuflhard, P., 1983. A semi-implicit mid-point rule for stiff systems of ordinary differential equations. Numer. Math. 41, 399–422.
Soo Kim, J, Park, J., Boong Kwon, O., Ju Lee, E., Han Yun, J., In Keel, S., 2008. Preferential diffusion effects in opposed-flow diffusion flame with blended fuels of CH4 and H2. Int. J. Hydrogen Energy 33 (2), 842–850.
Wu, Y., Al-Rahbi, I.S., Lu, Y., Kalghatgi, G.T., 2007. The stability of turbulent hydrogen jet flames with carbon dioxide and propane addition. Fuel 86 (12–13), 1840–1848.
Ilbas, M., Yilmaz, I., Kaplan, Y., 2005. Investigations of hydrogen and hydrogen-hydrocarbon composite fuel combustion and NOx emission characteristics in a model combustor. Int. J. Hydrogen Energy 30 (10), 1139–1147.
Burbano, H.J., Amell, A.A., García, J.M., 2008. Effects of hydrogen addition to methane on the flame structure and CO emissions in atmospheric burners. Int. J. Hydrogen Energy 33 (13), 3410–3415.
Guo, H., Smallwood, G.J., Liu, F., Ju, Y., Gülder, Ö.L., 2005. The effect of hydrogen addition on flammability limit and NOx emission in ultra-lean counterflow CH4/air premixed flames. Proc. Combust. Inst. 30 (1), 303–311.