

AN INTRODUCTION TO COMBUSTION

Concepts and Applications

THIRD EDITION

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From experimental measurements, the rate at which the fuel is consumed can be expressed as

$$\frac{d[X_F]}{dt} = -k_G(T)[X_F]^n[X_{Ox}]^m, \quad (4.2)$$

where the notation $[X_i]$ is used to denote the molar concentration (kmol/m^3 in SI units or gmol/cm^3 in CGS units) of the i th species in the mixture. Equation 4.2 states that the rate of disappearance of the fuel is proportional to each of the reactants raised to a power. The constant of proportionality, k_G , is called the **global rate coefficient**, and, in general, is not constant, but rather is a strong function of temperature. The minus sign indicates that the fuel concentration decreases with time. The exponents n and m relate to the **reaction order**. Equation 4.2 says that the reaction is n th order with respect to the fuel, m th order with respect to the oxidizer, and $(n + m)$ th order overall. For global reactions, n and m are not necessarily integers and arise from curvefitting experimental data. Later, we will see that for elementary reactions, reaction orders will always be integers. In general, a particular global expression in the form of Eqn. 4.2 holds only over a limited range of temperatures and pressures, and may depend on the details of the apparatus used to define the rate parameters. For example, different expressions for $k_G(T)$ and different values for n and m must be applied to cover a wide range of temperatures.

The use of global reactions to express the chemistry in a specific problem is frequently a “black box” approach. Although this approach may be useful in solving some problems, it does not provide a basis for understanding what is actually happening chemically in a system. For example, it is totally unrealistic to believe that a oxidizer molecules simultaneously collide with a single fuel molecule to form b product molecules, since this would require breaking several bonds and subsequently forming many new bonds. In reality, many sequential processes can occur involving many **intermediate species**. For example, consider the global reaction



To effect this global conversion of hydrogen and oxygen to water, the following **elementary reactions** are important:



among others.

In this partial mechanism for hydrogen combustion, we see from reaction 4.4 that when oxygen and hydrogen molecules collide and react, they do not yield water, but, instead, form the intermediate species HO_2 , the hydroperoxy radical, and a hydrogen atom, H , another radical. **Radicals** or **free radicals** are reactive molecules, or atoms, that have unpaired electrons. To form HO_2 from H_2 and O_2 ,

only one bond is broken and one bond formed. Alternatively, one might consider that H_2 and O_2 would react to form two hydroxyl radicals (OH); however, such a reaction is unlikely since it requires the breaking of two bonds and the creation of two new bonds. The hydrogen atom created in reaction 4.4 then reacts with O_2 to form two additional radicals, OH and O (reaction 4.5). It is the subsequent reaction (4.6) of the hydroxyl radical (OH) with molecular hydrogen that forms water. To have a complete picture of the combustion of H_2 and O_2 , more than 20 elementary reactions can be considered [1, 2]. These we consider in Chapter 5. The collection of elementary reactions necessary to describe an overall reaction is called a reaction **mechanism**. Reaction mechanisms may involve only a few steps (i.e., elementary reactions) or as many as several hundred. A field of active research involves selecting the minimum number of elementary steps necessary to describe a particular global reaction.

ELEMENTARY REACTION RATES

Bimolecular Reactions and Collision Theory

Most elementary reactions of interest in combustion are **bimolecular**; that is, two molecules collide and react to form two different molecules. For an arbitrary bimolecular reaction, this is expressed as



Reactions 4.4–4.6 are examples of bimolecular elementary reactions.

The rate at which the reaction proceeds is directly proportional to the concentrations (kmol/m^3) of the two reactant species, i.e.,

$$\frac{d[\text{A}]}{dt} = -k_{\text{bimolec}} [\text{A}][\text{B}]. \quad (4.9)$$

All elementary bimolecular reactions are overall second order, being first order with respect to each of the reacting species. The rate coefficient, k_{bimolec} , again is a function of temperature, but unlike the global rate coefficient, this rate coefficient has a theoretical basis. The SI units for k_{bimolec} are $\text{m}^3/\text{kmol}\cdot\text{s}$; however, much of the chemistry and combustion literature still uses CGS units.

Molecular collision theory can be used to provide insight into the form of Eqn. 4.9 and to suggest the temperature dependence of the bimolecular rate coefficient. As we will see, the collision theory for bimolecular reactions has many shortcomings; nevertheless, the approach is important for historical reasons and provides a way to visualize bimolecular reactions. In our discussion of molecular transport in Chapter 3, we introduced the concepts of wall collision frequency, mean molecular speed, and mean free path (Eqn. 3.10). These same concepts are important in our discussion of molecular collision rates. To determine the collision frequency of a pair of molecules, we start with the simpler case of a single molecule of diameter σ traveling with constant speed v and experiencing collisions with identical, but

Table 5.3 Chemical kinetic studies targeting real fuel combustion

Target Fuel	Surrogate Blend ¹	Reference	Comment
Natural gas	Methane (CH ₄) Ethane (C ₂ H ₆) Propane (C ₃ H ₈)	Dagaut [11]	—
Kerosene (Jet A-1)	<i>n</i> -Decane (C ₁₀ H ₂₂)	Dagaut [11]	Single-component model fuel
Kerosene (Jet A-1)	74% <i>n</i> -Decane (C ₁₀ H ₂₂) 15% <i>n</i> -Propylbenzene 11% <i>n</i> -Propylcyclohexane	Dagaut [11]	207 species and 1,592 reactions
Diesel fuel	36.5% <i>n</i> -Hexadecane (C ₁₆ H ₃₄) 24.5% Isooctane (C ₈ H ₁₈) 20.4% <i>n</i> -Propylcyclohexane 18.2% <i>n</i> -Propylbenzene	Dagaut [11]	298 species and 2,352 reactions
JP-8 (Jet fuel)	10% Isooctane 20% Methylcyclohexane (C ₇ H ₁₄) 15% <i>m</i> -Xylene (C ₈ H ₁₀) 30% <i>n</i> -Dodecane (C ₁₂ H ₂₆) 5% Tetralin (C ₁₀ H ₈) 20% Tetradecane (C ₁₄ H ₃₀)	Cooke <i>et al.</i> [12] Violi <i>et al.</i> [13] Ranzi <i>et al.</i> [14] Ranzi <i>et al.</i> [15] Ranzi <i>et al.</i> [16]	221 species and 5,032 reactions
Gasoline	Isooctane (neat) (C ₈ H ₁₈) Isooctane (C ₈ H ₁₈) – <i>n</i> -Heptane (C ₇ H ₁₆)	Curran <i>et al.</i> [17] Curran <i>et al.</i> [18]	Single-component model fuel and two-component surrogates; 860–990 species and 3,600–4,060 reactions
Gasoline	63–69% (liq. vol.) Isooctane (C ₈ H ₁₈) 14–20% (liq. vol.) Toluene (C ₇ H ₈) 17% (liq. vol.) <i>n</i> -Heptane (C ₇ H ₁₆) and 62% (liq. vol.) Isooctane (C ₈ H ₁₈) 20% (liq. vol.) Ethanol (C ₂ H ₅ OH) 18% (liq. vol.) <i>n</i> -Heptane (C ₇ H ₁₆) and 45% (liq. vol.) Toluene (C ₇ H ₈) 25% (liq. vol.) Isooctane (C ₈ H ₁₈) 20% (liq. vol.) <i>n</i> -Heptane (C ₇ H ₁₆) 10% (liq. vol.) Diisobutylene (C ₈ H ₁₆)	Andrae <i>et al.</i> [19] Andrae [20]	Octane numbers of blends match standard European gasoline.
Biodiesel	Methyl decaoate (C ₁₀ H ₂₂ O ₂ , i.e., CH ₃ (CH ₂) ₈ COOCH ₃)	Herbinet <i>et al.</i> [21]	3,012 species and 8,820 reactions

¹Compositions given in mole percent unless otherwise noted.

METHANE COMBUSTION

Complex Mechanism

Because of its unique tetrahedral molecular structure with large C–H bond energies, methane exhibits some unique combustion characteristics. For example, it has a high ignition temperature, low flame speed, and low reactivity in photochemical smog chemistry compared to other hydrocarbons.

Methane chemical kinetics are perhaps the most widely researched and, hence, most well understood. Kaufman [22], in a review of combustion kinetics indicated that the methane combustion mechanism evolved in the period 1970–1982 from less than 15 elementary steps with 12 species to 75 elementary steps, plus the 75 reverse reactions, with 25 species. More recently, several research groups have collaborated in the creation of an optimized methane kinetic mechanism [23]. This mechanism, designated GRI Mech, is based on the optimization techniques of Frenklach *et al.* [24]. GRI Mech [23] is available on the Internet and is continually updated. Version 3.0, shown in Table 5.4, considers 325 elementary reactions involving 53 species. Many of these steps we have seen before as part of the H₂ and CO oxidation mechanisms.

To make some sense of this complex system, we present reaction pathway analyses for both high-temperature and low-temperature combustion of CH₄ with air in a well-stirred reactor [25] using GRI Mech 2.11. A detailed discussion of the well-stirred reactor is presented in Chapter 6; however, for our purposes here, we need only recognize that reactions take place in a homogeneous, isothermal environment. The choice of a well-stirred reactor eliminates the need to account for a spatial distribution of species as would be encountered in a flame, for example.

Table 5.4 Complex methane combustion mechanism (GRI Mech 3.0) [23]

No.	Reaction	Forward Rate Coefficient ^a		
		A	b	E
C–H–O Reactions				
1	O + O + M → O ₂ + M	1.20E + 17	–1.0	0.0
2	O + H + M → OH + M	5.00E + 17	–1.0	0.0
3	O + H ₂ → H + OH	3.87E + 04	2.7	6,260
4	O + HO ₂ → OH + O ₂	2.00E + 13	0.0	0.0
5	O + H ₂ O ₂ → OH + HO ₂	9.63E + 06	2.0	4,000
6	O + CH → H + CO	5.70E + 13	0.0	0.0
7	O + CH ₂ → H + HCO	8.00E + 13	0.0	0.0
8 ^b	O + CH ₂ (S) → H ₂ + CO	1.50E + 13	0.0	0.0
9 ^b	O + CH ₂ (S) → H + HCO	1.50E + 13	0.0	0.0
10	O + CH ₃ → H + CH ₂ O	5.06E + 13	0.0	0.0
11	O + CH ₄ → OH + CH ₃	1.02E + 09	1.5	8,600
12	O + CO + M → CO ₂ + M	1.8E + 10	0.0	2,385
13	O + HCO → OH + CO	3.00E + 13	0.0	0.0
14	O + HCO → H + CO ₂	3.00E + 13	0.0	0.0
15	O + CH ₂ O → OH + HCO	3.90E + 13	0.0	3,540
16	O + CH ₂ OH → OH + CH ₂ O	1.00E + 13	0.0	0.0
17	O + CH ₃ O → OH + CH ₂ O	1.00E + 13	0.0	0.0
18	O + CH ₃ OH → OH + CH ₂ OH	3.88E + 05	2.5	3,100
19	O + CH ₃ OH → OH + CH ₃ O	1.30E + 05	2.5	5,000
20	O + C ₂ H → CH + CO	5.00E + 13	0.0	0.0
21	O + C ₂ H ₂ → H + HCCO	1.35E + 07	2.0	1,900
22	O + C ₂ H ₂ → OH + C ₂ H	4.60E + 19	–1.4	28,950
23	O + C ₂ H ₂ → CO + CH ₂	9.64E + 06	2.0	1,900
24	O + C ₂ H ₃ → H + CH ₂ CO	3.00E + 13	0.0	0.0

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient ^a		
		A	b	E
<i>C-H-O Reactions (continued)</i>				
25	$O + C_2H_4 \rightarrow CH_3 + HCO$	1.25E + 07	1.83	220
26	$O + C_2H_5 \rightarrow CH_3 + CH_2O$	2.24E + 13	0.0	0.0
27	$O + C_2H_6 \rightarrow OH + C_2H_5$	8.98E + 07	1.9	5,690
28	$O + HCCO \rightarrow H + CO + CO$	1.00E + 14	0.0	0.0
29	$O + CH_2CO \rightarrow OH + HCCO$	1.00E + 13	0.0	8,000
30	$O + CH_2CO \rightarrow CH_2 + CO_2$	1.75E + 12	0.0	1,350
31	$O_2 + CO \rightarrow O + CO_2$	2.50E + 12	0.0	47,800
32	$O_2 + CH_2O \rightarrow HO_2 + HCO$	1.00E + 14	0.0	40,000
33	$H + O_2 + M \rightarrow HO_2 + M$	2.80E + 18	-0.9	0.0
34	$H + O_2 + O_2 \rightarrow HO_2 + O_2$	2.08E + 19	-1.2	0.0
35	$H + O_2 + H_2O \rightarrow HO_2 + H_2O$	1.13E + 19	-0.8	0.0
36	$H + O_2 + N_2 \rightarrow HO_2 + N_2$	2.60E + 19	-1.2	0.0
37	$H + O_2 + Ar \rightarrow HO_2 + Ar$	7.00E + 17	-0.8	0.0
38	$H + O_2 \rightarrow O + OH$	2.65E + 16	-0.7	17,041
39	$H + H + M \rightarrow H_2 + M$	1.00E + 18	-1.0	0.0
40	$H + H + H_2 \rightarrow H_2 + H_2$	9.00E + 16	-0.6	0.0
41	$H + H + H_2O \rightarrow H_2 + H_2O$	6.00E + 19	-1.2	0.0
42	$H + H + CO_2 \rightarrow H_2 + CO_2$	5.50E + 20	-2.0	0.0
43	$H + OH + M \rightarrow H_2O + M$	2.20E + 22	-2.0	0.0
44	$H + HO_2 \rightarrow O + H_2O$	3.97E + 12	0.0	671
45	$H + HO_2 \rightarrow O_2 + H_2$	4.48E + 13	0.0	1,068
46	$H + HO_2 \rightarrow OH + OH$	8.4E + 13	0.0	635
47	$H + H_2O_2 \rightarrow HO_2 + H_2$	1.21E + 07	2.0	5,200
48	$H + H_2O_2 \rightarrow OH + H_2O$	1.00E + 13	0.0	3,600
49	$H + CH \rightarrow C + H_2$	1.65E + 14	0.0	0.0
50	$H + CH_2 (+ M) \rightarrow CH_3 (+ M)$		pressure dependent	
51 ^b	$H + CH_2(S) \rightarrow CH + H_2$	3.00E + 13	0.0	0.0
52	$H + CH_3 (+ M) \rightarrow CH_4 (+ M)$		pressure dependent	
53	$H + CH_4 \rightarrow CH_3 + H_2$	6.60E + 08	1.6	10,840
54	$H + HCO (+ M) \rightarrow CH_2O (+ M)$		pressure dependent	
55	$H + HCO \rightarrow H_2 + CO$	7.34E + 13	0.0	0.0
56	$H + CH_2O (+ M) \rightarrow CH_2OH (+ M)$		pressure dependent	
57	$H + CH_2O (+ M) \rightarrow CH_3O (+ M)$		pressure dependent	
58	$H + CH_2O \rightarrow HCO + H_2$	5.74E + 07	1.9	2,742
59	$H + CH_2OH (+ M) \rightarrow CH_3OH (+ M)$		pressure dependent	
60	$H + CH_2OH \rightarrow H_2 + CH_2O$	2.00E + 13	0.0	0.0
61	$H + CH_2OH \rightarrow OH + CH_3$	1.65E + 11	0.7	-284
62 ^b	$H + CH_2OH \rightarrow CH_2(S) + H_2O$	3.28E + 13	-0.1	610
63	$H + CH_3O (+ M) \rightarrow CH_3OH (+ M)$		pressure dependent	
64 ^b	$H + CH_2OH \rightarrow CH_2(S) + H_2O$	4.15E + 07	1.6	1,924
65	$H + CH_3O \rightarrow H_2 + CH_2O$	2.00E + 13	0.0	0.0
66	$H + CH_3O \rightarrow OH + CH_3$	1.50E + 12	0.5	-110
67 ^b	$H + CH_3O \rightarrow CH_2(S) + H_2O$	2.62E + 14	-0.2	1,070
68	$H + CH_3OH \rightarrow CH_2OH + H_2$	1.70E + 07	2.1	4,870
69	$H + CH_3OH \rightarrow CH_3O + H_2$	4.20E + 06	2.1	4,870
70	$H + C_2H (+ M) \rightarrow C_2H_2 (+ M)$		pressure dependent	

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient ^a		
		A	b	E
<i>C-H-O Reactions (continued)</i>				
71	$\text{H} + \text{C}_2\text{H}_2 (+ \text{M}) \rightarrow \text{C}_2\text{H}_3 (+ \text{M})$		pressure dependent	
72	$\text{H} + \text{C}_2\text{H}_3 (+ \text{M}) \rightarrow \text{C}_2\text{H}_4 (+ \text{M})$		pressure dependent	
73	$\text{H} + \text{C}_2\text{H}_3 \rightarrow \text{H}_2 + \text{C}_2\text{H}_2$	3.00E + 13	0.0	0.0
74	$\text{H} + \text{C}_2\text{H}_4 (+ \text{M}) \rightarrow \text{C}_2\text{H}_5 (+ \text{M})$		pressure dependent	
75	$\text{H} + \text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_3 + \text{H}_2$	1.32E + 06	2.5	12,240
76	$\text{H} + \text{C}_2\text{H}_5 (+ \text{M}) \rightarrow \text{C}_2\text{H}_6 (+ \text{M})$		pressure dependent	
77	$\text{H} + \text{C}_2\text{H}_5 \rightarrow \text{C}_2\text{H}_4 + \text{H}_2$	2.00E + 12	0.0	0.0
78	$\text{H} + \text{C}_2\text{H}_6 \rightarrow \text{C}_2\text{H}_5 + \text{H}_2$	1.15E + 08	1.9	7,530
79 ^b	$\text{H} + \text{HCCO} \rightarrow \text{CH}_3(\text{S}) + \text{CO}$	1.00E + 14	0.0	0.0
80	$\text{H} + \text{CH}_2\text{CO} \rightarrow \text{HCCO} + \text{H}_2$	5.00E + 13	0.0	8,000
81	$\text{H} + \text{CH}_2\text{CO} \rightarrow \text{CH}_3 + \text{CO}$	1.13E + 13	0.0	3,428
82	$\text{H} + \text{HCCOH} \rightarrow \text{H} + \text{CH}_2\text{CO}$	1.00E + 13	0.0	0.0
83	$\text{H}_2 + \text{CO} (+ \text{M}) \rightarrow \text{CH}_2\text{O} (+ \text{M})$		pressure dependent	
84	$\text{OH} + \text{H}_2 \rightarrow \text{H} + \text{H}_2\text{O}$	2.16E + 08	1.5	3,430
85	$\text{OH} + \text{OH} (+ \text{M}) \rightarrow \text{H}_2\text{O}_2 (+ \text{M})$		pressure dependent	
86	$\text{OH} + \text{OH} \rightarrow \text{O} + \text{H}_2\text{O}$	3.57E + 04	2.4	-2,110
87	$\text{OH} + \text{HO}_2 \rightarrow \text{O}_2 + \text{H}_2\text{O}$	1.45E + 13	0.0	-500
88	$\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2 + \text{H}_2\text{O}$	2.00E + 12	0.0	427
89	$\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2 + \text{H}_2\text{O}$	1.70E + 18	0.0	29,410
90	$\text{OH} + \text{C} \rightarrow \text{H} + \text{CO}$	5.00E + 13	0.0	0.0
91	$\text{OH} + \text{CH} \rightarrow \text{H} + \text{HCO}$	3.00E + 13	0.0	0.0
92	$\text{OH} + \text{CH}_2 \rightarrow \text{H} + \text{CH}_2\text{O}$	2.00E + 13	0.0	0.0
93	$\text{OH} + \text{CH}_2 \rightarrow \text{CH} + \text{H}_2\text{O}$	1.13E + 07	2.0	3,000
94 ^b	$\text{OH} + \text{CH}_2(\text{S}) \rightarrow \text{H} + \text{CH}_2\text{O}$	3.00E + 13	0.0	0.0
95	$\text{OH} + \text{CH}_3 (+ \text{M}) \rightarrow \text{CH}_3\text{OH} (+ \text{M})$		pressure dependent	
96	$\text{OH} + \text{CH}_3 \rightarrow \text{CH}_2 + \text{H}_2\text{O}$	5.60E + 07	1.6	5,420
97 ^b	$\text{OH} + \text{CH}_3 \rightarrow \text{CH}_2(\text{S}) + \text{H}_2\text{O}$	6.44E + 17	-1.3	1,417
98	$\text{OH} + \text{CH}_4 \rightarrow \text{CH}_3 + \text{H}_2\text{O}$	1.00E + 08	1.6	3,120
99	$\text{OH} + \text{CO} \rightarrow \text{H} + \text{CO}_2$	4.76E + 07	1.2	70
100	$\text{OH} + \text{HCO} \rightarrow \text{H}_2\text{O} + \text{CO}$	5.00E + 13	0.0	0.0
101	$\text{OH} + \text{CH}_2\text{O} \rightarrow \text{HCO} + \text{H}_2\text{O}$	3.43E + 09	1.2	-447
102	$\text{OH} + \text{CH}_2\text{OH} \rightarrow \text{H}_2\text{O} + \text{CH}_2\text{O}$	5.00E + 12	0.0	0.0
103	$\text{OH} + \text{CH}_3\text{O} \rightarrow \text{H}_2\text{O} + \text{CH}_2\text{O}$	5.00E + 12	0.0	0.0
104	$\text{OH} + \text{CH}_3\text{OH} \rightarrow \text{CH}_2\text{OH} + \text{H}_2\text{O}$	1.44E + 06	2.0	-840
105	$\text{OH} + \text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{O} + \text{H}_2\text{O}$	6.30E + 06	2.0	1,500
106	$\text{OH} + \text{C}_2\text{H} \rightarrow \text{H} + \text{HCCO}$	2.00E + 13	0.0	0.0
107	$\text{OH} + \text{C}_2\text{H}_2 \rightarrow \text{H} + \text{CH}_2\text{CO}$	2.18E - 04	4.5	-1,000
108	$\text{OH} + \text{C}_2\text{H}_2 \rightarrow \text{H} + \text{HCCOH}$	5.04E + 05	2.3	13,500
109	$\text{OH} + \text{C}_2\text{H}_2 \rightarrow \text{C}_2\text{H} + \text{H}_2\text{O}$	3.37E + 07	2.0	14,000
110	$\text{OH} + \text{C}_2\text{H}_2 \rightarrow \text{CH}_3 + \text{CO}$	4.83E - 04	4.0	-2,000
111	$\text{OH} + \text{C}_2\text{H}_3 \rightarrow \text{H}_2\text{O} + \text{C}_2\text{H}_2$	5.00E + 12	0.0	0.0
112	$\text{OH} + \text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_3 + \text{H}_2\text{O}$	3.60E + 06	2.0	2,500
113	$\text{OH} + \text{C}_2\text{H}_6 \rightarrow \text{C}_2\text{H}_5 + \text{H}_2\text{O}$	3.54E + 06	2.1	870
114	$\text{OH} + \text{CH}_2\text{CO} \rightarrow \text{HCCO} + \text{H}_2\text{O}$	7.50E + 12	0.0	2,000
115	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{O}_2 + \text{H}_2\text{O}_2$	1.30E + 11	0.0	-1,630
116	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{O}_2 + \text{H}_2\text{O}_2$	4.20E + 14	0.0	12,000

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient ^a		
		A	b	E
<i>C-H-O Reactions (continued)</i>				
117	$\text{HO}_2 + \text{CH}_2 \rightarrow \text{OH} + \text{CH}_2\text{O}$	2.00E + 13	0.0	0.0
118	$\text{HO}_2 + \text{CH}_3 \rightarrow \text{O}_2 + \text{CH}_4$	1.00E + 12	0.0	0.0
119	$\text{HO}_2 + \text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{O}$	3.78E + 13	0.0	0.0
120	$\text{HO}_2 + \text{CO} \rightarrow \text{OH} + \text{CO}_2$	1.50E + 14	0.0	23,600
121	$\text{HO}_2 + \text{CH}_2\text{O} \rightarrow \text{HCO} + \text{H}_2\text{O}_2$	5.60E + 06	2.0	12,000
122	$\text{C} + \text{O}_2 \rightarrow \text{O} + \text{CO}$	5.80E + 13	0.0	576
123	$\text{C} + \text{CH}_2 \rightarrow \text{H} + \text{C}_2\text{H}$	5.00E + 13	0.0	0.0
124	$\text{C} + \text{CH}_3 \rightarrow \text{H} + \text{C}_2\text{H}_2$	5.00E + 13	0.0	0.0
125	$\text{CH} + \text{O}_2 \rightarrow \text{O} + \text{HCO}$	6.71E + 13	0.0	0.0
126	$\text{CH} + \text{H}_2 \rightarrow \text{H} + \text{CH}_2$	1.08E + 14	0.0	3,110
127	$\text{CH} + \text{H}_2\text{O} \rightarrow \text{H} + \text{CH}_2\text{O}$	5.71E + 12	0.0	-755
128	$\text{CH} + \text{CH}_2 \rightarrow \text{H} + \text{C}_2\text{H}_2$	4.00E + 13	0.0	0.0
129	$\text{CH} + \text{CH}_3 \rightarrow \text{H} + \text{C}_2\text{H}_3$	3.00E + 13	0.0	0.0
130	$\text{CH} + \text{CH}_4 \rightarrow \text{H} + \text{C}_2\text{H}_4$	6.00E + 13	0.0	0.0
131	$\text{CH} + \text{CO} (+ \text{M}) \rightarrow \text{HCCO} (+ \text{M})$		pressure dependent	
132	$\text{CH} + \text{CO}_2 \rightarrow \text{HCO} + \text{CO}$	1.90E + 14	0.0	15,792
133	$\text{CH} + \text{CH}_2\text{O} \rightarrow \text{H} + \text{CH}_2\text{CO}$	9.46E + 13	0.0	-515
134	$\text{CH} + \text{HCCO} \rightarrow \text{CO} + \text{C}_2\text{H}_2$	5.00E + 13	0.0	0.0
135	$\text{CH}_2 + \text{O}_2 \rightarrow \text{OH} + \text{HCO}$	5.00E + 12	0.0	1,500
136	$\text{CH}_2 + \text{H}_2 \rightarrow \text{H} + \text{CH}_3$	5.00E + 05	2.0	7,230
137	$\text{CH}_2 + \text{CH}_2 \rightarrow \text{H}_2 + \text{C}_2\text{H}_2$	1.60E + 15	0.0	11,944
138	$\text{CH}_2 + \text{CH}_3 \rightarrow \text{H} + \text{C}_2\text{H}_4$	4.00E + 13	0.0	0.0
139	$\text{CH}_2 + \text{CH}_4 \rightarrow \text{CH}_3 + \text{CH}_3$	2.46E + 06	2.0	8,270
140	$\text{CH}_2 + \text{CO} (+ \text{M}) \rightarrow \text{CH}_2\text{CO} (+ \text{M})$		pressure dependent	
141	$\text{CH}_2 + \text{HCCO} \rightarrow \text{C}_2\text{H}_3 + \text{CO}$	3.00E + 13	0.0	0.0
142 ^b	$\text{CH}_2(\text{S}) + \text{N}_2 \rightarrow \text{CH}_2 + \text{N}_2$	1.50E + 13	0.0	600
143 ^b	$\text{CH}_2(\text{S}) + \text{Ar} \rightarrow \text{CH}_2 + \text{Ar}$	9.00E + 12	0.0	600
144 ^b	$\text{CH}_2(\text{S}) + \text{O}_2 \rightarrow \text{H} + \text{OH} + \text{CO}$	2.80E + 13	0.0	0.0
145 ^b	$\text{CH}_2(\text{S}) + \text{O}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$	1.20E + 13	0.0	0.0
146 ^b	$\text{CH}_2(\text{S}) + \text{H}_2 \rightarrow \text{CH}_3 + \text{H}$	7.00E + 13	0.0	0.0
147 ^b	$\text{CH}_2(\text{S}) + \text{H}_2\text{O} (+ \text{M}) \rightarrow \text{CH}_3\text{OH} (+ \text{M})$		pressure dependent	
148 ^b	$\text{CH}_2(\text{S}) + \text{H}_2\text{O} \rightarrow \text{CH}_2 + \text{H}_2\text{O}$	3.00E + 13	0.0	0.0
149 ^b	$\text{CH}_2(\text{S}) + \text{CH}_3 \rightarrow \text{H} + \text{C}_2\text{H}_4$	1.20E + 13	0.0	-570
150 ^b	$\text{CH}_2(\text{S}) + \text{CH}_4 \rightarrow \text{CH}_3 + \text{CH}_3$	1.60E + 13	0.0	-570
151 ^b	$\text{CH}_2(\text{S}) + \text{CO} \rightarrow \text{CH}_2 + \text{CO}$	9.00E + 12	0.0	0.0
152 ^b	$\text{CH}_2(\text{S}) + \text{CO}_2 \rightarrow \text{CH}_2 + \text{CO}_2$	7.00E + 12	0.0	0.0
153 ^b	$\text{CH}_2(\text{S}) + \text{CO}_2 \rightarrow \text{CO} + \text{CH}_2\text{O}$	1.40E + 13	0.0	0.0
154 ^b	$\text{CH}_2(\text{S}) + \text{C}_2\text{H}_6 \rightarrow \text{CH}_3 + \text{C}_2\text{H}_5$	4.00E + 13	0.0	-550
155	$\text{CH}_3 + \text{O}_2 \rightarrow \text{O} + \text{CH}_3\text{O}$	3.56E + 13	0.0	30,480
156	$\text{CH}_3 + \text{O}_2 \rightarrow \text{OH} + \text{CH}_2\text{O}$	2.31E + 12	0.0	20,315
157	$\text{CH}_3 + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2 + \text{CH}_4$	2.45E + 04	2.47	5,180
158	$\text{CH}_3 + \text{CH}_3 (+ \text{M}) \rightarrow \text{C}_2\text{H}_6 (+ \text{M})$		pressure dependent	
159	$\text{CH}_3 + \text{CH}_3 \rightarrow \text{H} + \text{C}_2\text{H}_5$	6.48E + 12	0.1	10,600
160	$\text{CH}_3 + \text{HCO} \rightarrow \text{CH}_4 + \text{CO}$	2.65E + 13	0.0	0.0
161	$\text{CH}_3 + \text{CH}_2\text{O} \rightarrow \text{HCO} + \text{CH}_4$	3.32E + 03	2.8	5,860

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient ^a		
		A	b	E
<i>C-H-O Reactions (continued)</i>				
162	$\text{CH}_3 + \text{CH}_3\text{OH} \rightarrow \text{CH}_2\text{OH} + \text{CH}_4$	3.00E + 07	1.5	9,940
163	$\text{CH}_3 + \text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{O} + \text{CH}_4$	1.00E + 07	1.5	9,940
164	$\text{CH}_3 + \text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_3 + \text{CH}_4$	2.27E + 05	2.0	9,200
165	$\text{CH}_3 + \text{C}_2\text{H}_6 \rightarrow \text{C}_2\text{H}_5 + \text{CH}_4$	6.14E + 06	1.7	10,450
166	$\text{HCO} + \text{H}_2\text{O} \rightarrow \text{H} + \text{CO} + \text{H}_2\text{O}$	1.55E + 18	-1.0	17,000
167	$\text{HCO} + \text{M} \rightarrow \text{H} + \text{CO} + \text{M}$	1.87E + 17	-1.0	17,000
168	$\text{HCO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{CO}$	1.35E + 13	0.0	400
169	$\text{CH}_2\text{OH} + \text{O}_2 \rightarrow \text{HO}_2 + \text{CH}_2\text{O}$	1.80E + 13	0.0	900
170	$\text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{HO}_2 + \text{CH}_2\text{O}$	4.28E - 13	7.6	-3,530
171	$\text{C}_2\text{H} + \text{O}_2 \rightarrow \text{HCO} + \text{CO}$	1.00E + 13	0.0	-755
172	$\text{C}_2\text{H} + \text{H}_2 \rightarrow \text{H} + \text{C}_2\text{H}_2$	5.68E + 10	0.9	1,993
173	$\text{C}_2\text{H}_3 + \text{O}_2 \rightarrow \text{HCO} + \text{CH}_2\text{O}$	4.58E + 16	-1.4	1,015
174	$\text{C}_2\text{H}_4 (+ \text{M}) \rightarrow \text{H}_2 + \text{C}_2\text{H}_2 (+ \text{M})$		pressure dependent	
175	$\text{C}_2\text{H}_3 + \text{O}_2 \rightarrow \text{HO}_2 + \text{C}_2\text{H}_4$	8.40E + 11	0.0	3,875
176	$\text{HCCO} + \text{O}_2 \rightarrow \text{OH} + \text{CO} + \text{CO}$	3.20E + 12	0.0	854
177	$\text{HCCO} + \text{HCCO} \rightarrow \text{CO} + \text{CO} + \text{C}_2\text{H}_2$	1.00E + 13	0.0	0.0
<i>N-Containing Reactions</i>				
178	$\text{N} + \text{NO} \rightarrow \text{N}_2 + \text{O}$	2.70E + 13	0.0	355
179	$\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$	9.00E + 09	1.0	6,500
180	$\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$	3.36E + 13	0.0	385
181	$\text{N}_2\text{O} + \text{O} \rightarrow \text{N}_2 + \text{O}_2$	1.40E + 12	0.0	10,810
182	$\text{N}_2\text{O} + \text{O} \rightarrow \text{NO} + \text{NO}$	2.90E + 13	0.0	23,150
183	$\text{N}_2\text{O} + \text{H} \rightarrow \text{N}_2 + \text{OH}$	3.87E + 14	0.0	18,880
184	$\text{N}_2\text{O} + \text{OH} \rightarrow \text{N}_2 + \text{HO}_2$	2.00E + 12	0.0	21,060
185	$\text{N}_2\text{O} (+ \text{M}) \rightarrow \text{N}_2 + \text{O} (+ \text{M})$		pressure dependent	
186	$\text{HO}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{OH}$	2.11E + 12	0.0	-480
187	$\text{NO} + \text{O} + \text{M} \rightarrow \text{NO}_2 + \text{M}$	1.06E + 20	-1.4	0.0
188	$\text{NO}_2 + \text{O} \rightarrow \text{NO} + \text{O}_2$	3.90E + 12	0.0	-240
189	$\text{NO}_2 + \text{H} \rightarrow \text{NO} + \text{OH}$	1.32E + 14	0.0	360
190	$\text{NH} + \text{O} \rightarrow \text{NO} + \text{H}$	4.00E + 13	0.0	0.0
191	$\text{NH} + \text{H} \rightarrow \text{N} + \text{H}_2$	3.20E + 13	0.0	330
192	$\text{NH} + \text{OH} \rightarrow \text{HNO} + \text{H}$	2.00E + 13	0.0	0.0
193	$\text{NH} + \text{OH} \rightarrow \text{N} + \text{H}_2\text{O}$	2.00E + 09	1.2	0.0
194	$\text{NH} + \text{O}_2 \rightarrow \text{HNO} + \text{O}$	4.61E + 05	2.0	6,500
195	$\text{NH} + \text{O}_2 \rightarrow \text{NO} + \text{OH}$	1.28E + 06	1.5	100
196	$\text{NH} + \text{N} \rightarrow \text{N}_2 + \text{H}$	1.50E + 13	0.0	0.0
197	$\text{NH} + \text{H}_2\text{O} \rightarrow \text{HNO} + \text{H}_2$	2.00E + 13	0.0	13,850
198	$\text{NH} + \text{NO} \rightarrow \text{N}_2 + \text{OH}$	2.16E + 13	-0.2	0.0
199	$\text{NH} + \text{NO} \rightarrow \text{N}_2\text{O} + \text{H}$	3.65E + 14	-0.5	0.0
200	$\text{NH}_2 + \text{O} \rightarrow \text{OH} + \text{NH}$	3.00E + 12	0.0	0.0

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient ^a		
		A	b	E
<i>N-Containing Reactions (continued)</i>				
201	$\text{NH}_2 + \text{O} \rightarrow \text{H} + \text{HNO}$	3.9E + 13	0.0	0.0
202	$\text{NH}_2 + \text{H} \rightarrow \text{NH} + \text{H}_2$	4.00E + 13	0.0	3,650
203	$\text{NH}_2 + \text{OH} \rightarrow \text{NH} + \text{H}_2\text{O}$	9.00E + 07	1.5	-460
204	$\text{NNH} \rightarrow \text{N}_2 + \text{H}$	3.30E + 08	0.0	0.0
205	$\text{NNH} + \text{M} \rightarrow \text{N}_2 + \text{H} + \text{M}$	1.30E + 14	-0.1	4,980
206	$\text{NNH} + \text{O}_2 \rightarrow \text{HO}_2 + \text{N}_2$	5.00E + 12	0.0	0.0
207	$\text{NNH} + \text{O} \rightarrow \text{OH} + \text{N}_2$	2.50E + 13	0.0	0.0
208	$\text{NNH} + \text{O} \rightarrow \text{NH} + \text{NO}$	7.00E + 13	0.0	0.0
209	$\text{NNH} + \text{H} \rightarrow \text{H}_2 + \text{N}_2$	5.00E + 13	0.0	0.0
210	$\text{NNH} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{N}_2$	2.00E + 13	0.0	0.0
211	$\text{NNH} + \text{CH}_3 \rightarrow \text{CH}_4 + \text{N}_2$	2.50E + 13	0.0	0.0
212	$\text{H} + \text{NO} + \text{M} \rightarrow \text{HNO} + \text{M}$	4.48E + 19	-1.3	740
213	$\text{HNO} + \text{O} \rightarrow \text{NO} + \text{OH}$	2.50E + 13	0.0	0.0
214	$\text{HNO} + \text{H} \rightarrow \text{H}_2 + \text{NO}$	9.00E + 11	0.7	660
215	$\text{HNO} + \text{OH} \rightarrow \text{NO} + \text{H}_2\text{O}$	1.30E + 07	1.9	-950
216	$\text{HNO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{NO}$	1.00E + 13	0.0	13,000
217	$\text{CN} + \text{O} \rightarrow \text{CO} + \text{N}$	7.70E + 13	0.0	0.0
218	$\text{CN} + \text{OH} \rightarrow \text{NCO} + \text{H}$	4.00E + 13	0.0	0.0
219	$\text{CN} + \text{H}_2\text{O} \rightarrow \text{HCN} + \text{OH}$	8.00E + 12	0.0	7,460
220	$\text{CN} + \text{O}_2 \rightarrow \text{NCO} + \text{O}$	6.14E + 12	0.0	-440
221	$\text{CN} + \text{H}_2 \rightarrow \text{HCN} + \text{H}$	2.95E + 05	2.5	2,240
222	$\text{NCO} + \text{O} \rightarrow \text{NO} + \text{CO}$	2.35E + 13	0.0	0.0
223	$\text{NCO} + \text{H} \rightarrow \text{NH} + \text{CO}$	5.40E + 13	0.0	0.0
224	$\text{NCO} + \text{OH} \rightarrow \text{NO} + \text{H} + \text{CO}$	2.50E + 12	0.0	0.0
225	$\text{NCO} + \text{N} \rightarrow \text{N}_2 + \text{CO}$	2.00E + 13	0.0	0.0
226	$\text{NCO} + \text{O}_2 \rightarrow \text{NO} + \text{CO}_2$	2.00E + 12	0.0	20,000
227	$\text{NCO} + \text{M} \rightarrow \text{N} + \text{CO} + \text{M}$	3.10E + 14	0.0	54,050
228	$\text{NCO} + \text{NO} \rightarrow \text{N}_2\text{O} + \text{CO}$	1.90E + 17	-1.5	740
229	$\text{NCO} + \text{NO} \rightarrow \text{N}_2 + \text{CO}_2$	3.80E + 18	-2.0	800
230	$\text{HCN} + \text{M} \rightarrow \text{H} + \text{CN} + \text{M}$	1.04E + 29	-3.3	126,600
231	$\text{HCN} + \text{O} \rightarrow \text{NCO} + \text{H}$	2.03E + 04	2.6	4,980
232	$\text{HCN} + \text{O} \rightarrow \text{NH} + \text{CO}$	5.07E + 03	2.6	4,980
233	$\text{HCN} + \text{O} \rightarrow \text{CN} + \text{OH}$	3.91E + 09	1.6	26,600
234	$\text{HCN} + \text{OH} \rightarrow \text{HOCN} + \text{H}$	1.10E + 06	2.0	13,370
235	$\text{HCN} + \text{OH} \rightarrow \text{HNCO} + \text{H}$	4.40E + 03	2.3	6,400
236	$\text{HCN} + \text{OH} \rightarrow \text{NH}_2 + \text{CO}$	1.60E + 02	2.6	9,000
237	$\text{H} + \text{HCN} + \text{M} \rightarrow \text{H}_2\text{CN} + \text{M}$		pressure dependent	
238	$\text{H}_2\text{CN} + \text{N} \rightarrow \text{N}_2 + \text{CH}_2$	6.00E + 13	0.0	400
239	$\text{C} + \text{N}_2 \rightarrow \text{CN} + \text{N}$	6.30E + 13	0.0	46,020
240	$\text{CH} + \text{N}_2 \rightarrow \text{HCN} + \text{N}$	3.12E + 09	0.9	20,130
241	$\text{CH} + \text{N}_2 (+ \text{M}) \rightarrow \text{HCNN} (+ \text{M})$		pressure dependent	
242	$\text{CH}_2 + \text{N}_2 \rightarrow \text{HCN} + \text{NH}$	1.00E + 13	0.0	74,000
243 ^b	$\text{CH}_2(\text{S}) + \text{N}_2 \rightarrow \text{NH} + \text{HCN}$	1.00E + 11	0.0	65,000

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient ^a		
		A	b	E
<i>N-Containing Reactions (continued)</i>				
244	C + NO → CN + O	1.90E + 13	0.0	0.0
245	C + NO → CO + N	2.90E + 13	0.0	0.0
246	CH + NO → HCN + O	4.10E + 13	0.0	0.0
247	CH + NO → H + NCO	1.62E + 13	0.0	0.0
248	CH + NO → N + HCO	2.46E + 13	0.0	0.0
249	CH ₂ + NO → H + HNCO	3.10E + 17	-1.4	1,270
250	CH ₂ + NO → OH + HCN	2.90E + 14	-0.7	760
251	CH ₂ + NO → H + HCNO	3.80E + 13	-0.4	580
252 ^b	CH ₂ (S) + NO → H + HNCO	3.10E + 17	-1.4	1,270
253 ^b	CH ₂ (S) + NO → OH + HCN	2.90E + 14	-0.7	760
254 ^b	CH ₂ (S) + NO → H + HCNO	3.80E + 13	-0.4	580
255	CH ₃ + NO → HCN + H ₂ O	9.60E + 13	0.0	28,800
256	CH ₃ + NO → H ₂ CN + OH	1.00E + 12	0.0	21,750
257	HCNN + O → CO + H + N ₂	2.20E + 13	0.0	0.0
258	HCNN + O → HCN + NO	2.00E + 12	0.0	0.0
259	HCNN + O ₂ → O + HCO + N ₂	1.20E + 13	0.0	0.0
260	HCNN + OH → H + HCO + N ₂	1.20E + 13	0.0	0.0
261	HCNN + H → CH ₂ + N ₂	1.00E + 14	0.0	0.0
262	HNCO + O → NH + CO ₂	9.80E + 07	1.4	8,500
263	HNCO + O → HNO + CO	1.50E + 08	1.6	44,000
264	HNCO + O → NCO + OH	2.20E + 06	2.1	11,400
265	HNCO + H → NH ₂ + CO	2.25E + 07	1.7	3,800
266	HNCO + H → H ₂ + NCO	1.05E + 05	2.5	13,300
267	HNCO + OH → NCO + H ₂ O	3.30E + 07	1.5	3,600
268	HNCO + OH → NH ₂ + CO ₂	3.30E + 06	1.5	3,600
269	HNCO + M → NH + CO + M	1.18E + 16	0.0	84,720
270	HCNO + H → H + HNCO	2.10E + 15	-0.7	2,850
271	HCNO + H → OH + HCN	2.70E + 11	0.2	2,120
272	HCNO + H → NH ₂ + CO	1.70E + 14	-0.8	2,890
273	HOCN + H → H + HNCO	2.00E + 07	2.0	2,000
274	HCCO + NO → HCNO + CO	9.00E + 12	0.0	0.0
275	CH ₃ + N → H ₂ CN + H	6.10E + 14	-0.3	290
276	CH ₃ + N → HCN + H ₂	3.70E + 12	0.1	-90
277	NH ₃ + H → NH ₂ + H ₂	5.40E + 05	2.4	9,915
278	NH ₃ + OH → NH ₂ + H ₂ O	5.00E + 07	1.6	955
279	NH ₃ + O → NH ₂ + OH	9.40E + 06	1.9	6,460
<i>Reactions Added in Update from Version 2.11 to Version 3.0</i>				
280	NH + CO ₂ → HNO + CO	1.00E + 13	0.0	14,350
281	CN + NO ₂ → NCO + NO	6.16E + 15	-0.8	345
282	NCO + NO ₂ → N ₂ O + CO ₂	3.25E + 12	0.0	-705
283	N + CO ₂ → NO + CO	3.00E + 12	0.0	11,300
284	O + CH ₃ → H + H ₂ + CO	3.37E + 13	0.0	0.0
285	O + C ₂ H ₄ → CH ₂ CHO	6.70E + 06	1.8	220
286	O + C ₂ H ₅ → H + CH ₃ CHO	1.10E + 14	0.0	0.0

Table 5.4 (continued)

No.	Reaction	Forward Rate Coefficient ^a		
		A	b	E
<i>Reactions Added in Update from Version 2.11 to Version 3.0 (continued)</i>				
287	$\text{OH} + \text{HO}_2 \rightarrow \text{O}_2 + \text{H}_2\text{O}$	5.00E + 15	0.0	17,330
288	$\text{OH} + \text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_2\text{O}$	8.00E + 09	0.5	-1,755
289	$\text{CH} + \text{H}_2 + \text{M} \rightarrow \text{CH}_3 + \text{M}$		pressure dependent	
290	$\text{CH}_2 + \text{O}_2 \rightarrow \text{H} + \text{H} + \text{CO}_2$	5.80E + 12	0.0	1,500
291	$\text{CH}_2 + \text{O}_2 \rightarrow \text{O} + \text{CH}_2\text{O}$	2.40E + 12	0.0	1,500
292	$\text{CH}_2 + \text{CH}_2 \rightarrow \text{H} + \text{H} + \text{C}_2\text{H}_2$	2.00E + 14	0.0	10,989
293 ^b	$\text{CH}_2(\text{S}) + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{CH}_2\text{O}$	6.82E + 10	0.2	-935
294	$\text{C}_2\text{H}_3 + \text{O}_2 \rightarrow \text{O} + \text{CH}_2\text{CHO}$	3.03E + 11	0.3	11
295	$\text{C}_2\text{H}_3 + \text{O}_2 \rightarrow \text{HO}_2 + \text{C}_2\text{H}_2$	1.34E + 06	1.6	-384
296	$\text{O} + \text{CH}_3\text{CHO} \rightarrow \text{OH} + \text{CH}_2\text{CHO}$	2.92E + 12	0.0	1,808
297	$\text{O} + \text{CH}_3\text{CHO} \rightarrow \text{OH} + \text{CH}_3 + \text{CO}$	2.92E + 12	0.0	1,808
298	$\text{O}_2 + \text{CH}_3\text{CHO} \rightarrow \text{HO}_2 + \text{CH}_3 + \text{CO}$	3.01E + 13	0.0	39,150
299	$\text{H} + \text{CH}_3\text{CHO} \rightarrow \text{CH}_2\text{CHO} + \text{H}_2$	2.05E + 09	1.2	2,405
300	$\text{H} + \text{CH}_3\text{CHO} \rightarrow \text{CH}_3 + \text{H}_2 + \text{CO}$	2.05E + 09	1.2	2,405
301	$\text{OH} + \text{CH}_3\text{CHO} \rightarrow \text{CH}_3 + \text{H}_2\text{O} + \text{CO}$	2.34E + 10	0.7	-1,113
302	$\text{HO}_2 + \text{CH}_3\text{CHO} \rightarrow \text{CH}_3 + \text{H}_2\text{O}_2 + \text{CO}$	3.01E + 12	0.0	11,923
303	$\text{CH}_3 + \text{CH}_3\text{CHO} \rightarrow \text{CH}_3 + \text{CH}_4 + \text{CO}$	2.72E + 06	1.8	5,920
304	$\text{H} + \text{CH}_2\text{CO} + \text{M} \rightarrow \text{CH}_2\text{CHO} + \text{M}$		pressure dependent	
305	$\text{O} + \text{CH}_2\text{CHO} \rightarrow \text{H} + \text{CH}_2 + \text{CO}_2$	1.50E + 14	0.0	0.0
306	$\text{O}_2 + \text{CH}_2\text{CHO} \rightarrow \text{OH} + \text{CO} + \text{CH}_2\text{O}$	1.81E + 10	0.0	0.0
307	$\text{O}_2 + \text{CH}_2\text{CHO} \rightarrow \text{OH} + \text{HCO} + \text{HCO}$	2.35E + 10	0.0	0.0
308	$\text{H} + \text{CH}_2\text{CHO} \rightarrow \text{CH}_3 + \text{HCO}$	2.20E + 13	0.0	0.0
309	$\text{H} + \text{CH}_2\text{CHO} \rightarrow \text{CH}_2\text{CO} + \text{H}_2$	1.10E + 13	0.0	0.0
310	$\text{OH} + \text{CH}_2\text{CHO} \rightarrow \text{H}_2\text{O} + \text{CH}_2\text{CO}$	1.20E + 13	0.0	0.0
311	$\text{OH} + \text{CH}_2\text{CHO} \rightarrow \text{HCO} + \text{CH}_2\text{OH}$	3.01E + 13	0.0	0.0
312	$\text{CH}_3 + \text{C}_2\text{H}_5 + \text{M} \rightarrow \text{C}_3\text{H}_8 + \text{M}$		pressure dependent	
313	$\text{O} + \text{C}_3\text{H}_8 \rightarrow \text{OH} + \text{C}_3\text{H}_7$	1.93E + 05	2.7	3,716
314	$\text{H} + \text{C}_3\text{H}_8 \rightarrow \text{C}_3\text{H}_7 + \text{H}_2$	1.32E + 06	2.5	6,756
315	$\text{OH} + \text{C}_3\text{H}_8 \rightarrow \text{C}_3\text{H}_7 + \text{H}_2\text{O}$	3.16E + 07	1.8	934
316	$\text{C}_3\text{H}_7 + \text{H}_2\text{O}_2 \rightarrow \text{HO}_2 + \text{C}_3\text{H}_8$	3.78E + 02	2.7	1,500
317	$\text{CH}_3 + \text{C}_3\text{H}_8 \rightarrow \text{C}_3\text{H}_7 + \text{CH}_4$	9.03E - 01	3.6	7,154
318	$\text{CH}_3 + \text{C}_2\text{H}_4 + \text{M} \rightarrow \text{C}_3\text{H}_7 + \text{M}$		pressure dependent	
319	$\text{O} + \text{C}_3\text{H}_7 \rightarrow \text{C}_2\text{H}_5 + \text{CH}_2\text{O}$	9.64E + 13	0.0	0.0
320	$\text{H} + \text{C}_3\text{H}_7 + \text{M} \rightarrow \text{C}_3\text{H}_8 + \text{M}$		pressure dependent	
321	$\text{H} + \text{C}_3\text{H}_7 \rightarrow \text{CH}_3 + \text{C}_2\text{H}_5$	4.06E + 06	2.2	890
322	$\text{OH} + \text{C}_3\text{H}_7 \rightarrow \text{C}_2\text{H}_5 + \text{CH}_2\text{OH}$	2.41E + 13	0.0	0.0
323	$\text{HO}_2 + \text{C}_3\text{H}_7 \rightarrow \text{O}_2 + \text{C}_3\text{H}_8$	2.55E + 10	0.3	-943
324	$\text{HO}_2 + \text{C}_3\text{H}_7 \rightarrow \text{OH} + \text{C}_2\text{H}_5 + \text{CH}_2\text{O}$	2.41E + 13	0.0	0.0
325	$\text{CH}_3 + \text{C}_3\text{H}_7 \rightarrow \text{C}_2\text{H}_5 + \text{C}_2\text{H}_5$	1.93E + 13	-0.3	0.0

^aThe forward rate coefficient $k = A T^b \exp(-E/RT)$. R is the universal gas constant, T is the temperature in K. The units of A involve gmol/cm^3 and s , and those of E , cal/gmol .

^b $\text{CH}_2(\text{S})$ designates the singlet state of CH_2 .

Laminar Premixed Flames

OVERVIEW

In previous chapters, we introduced the concepts of mass transfer (Chapter 3) and chemical kinetics (Chapters 4 and 5) and linked them with familiar thermodynamic and heat transfer concepts in Chapters 6 and 7. Understanding premixed laminar flames requires us to utilize all of these concepts. Our development in Chapter 7 of the one-dimensional conservation equations for a reacting flow will be the starting point for analyzing laminar flames.

Laminar premixed flames, frequently in conjunction with diffusion flames, have application in many residential, commercial, and industrial devices and processes. Examples include gas ranges and ovens, heating appliances, and Bunsen burners. An advanced cooktop burner for a gas range is illustrated in Fig. 8.1. Laminar, premixed, natural-gas flames also are frequently employed in the manufacturing of glass products. As suggested by the examples given above, laminar premixed flames are by themselves important; but, perhaps more importantly, understanding laminar flames is a necessary prerequisite to the study of turbulent flames. In both laminar and turbulent flows, the same physical processes are active, and many turbulent flame theories are based on an underlying laminar flame structure. In this chapter, we will qualitatively describe the essential characteristics of laminar premixed flames and develop a simplified analysis of these flames that allows us to see what factors influence the laminar flame speed and the flame thickness. A detailed analysis using state-of-the-art methods will illustrate the power of numerical simulations in understanding flame structure. We will also examine experimental data that illustrate how equivalence ratio, temperature, pressure, and fuel type affect flame speed and flame thickness. Flame speed is emphasized because it is this property that dictates flame shape and important flame-stability characteristics, such as blowoff and flashback. The chapter concludes with discussion of flammability limits and ignition and extinction phenomena.

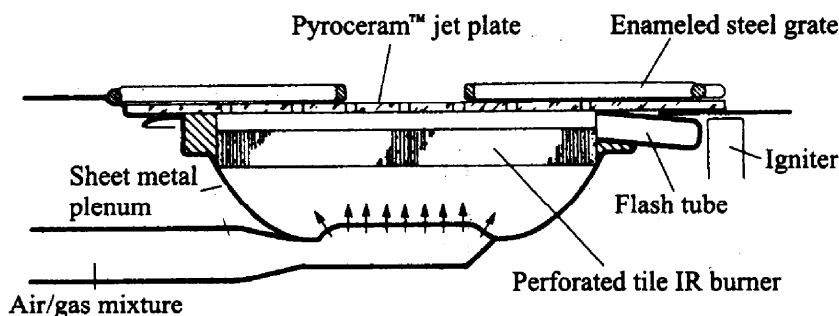


Figure 8.1 Advanced residential cooktop burner for gas ranges.
 | SOURCE: Courtesy of the Gas Research Institute.

PHYSICAL DESCRIPTION

Definition

Before proceeding, it is useful to define what we mean by a flame. A **flame** is a self-sustaining propagation of a localized combustion zone at subsonic velocities. There are several key words in this definition. First, we require a flame to be localized; that is, the flame occupies only a small portion of the combustible mixture at any one time. This is in contrast to the various homogeneous reactors we studied in Chapter 6, where reaction was assumed to occur uniformly throughout the reaction vessel. The second key word is subsonic. A discrete combustion wave that travels subsonically is termed a **deflagration**. It is also possible for combustion waves to propagate at supersonic velocities. Such a wave is called a **detonation**. The fundamental propagation mechanisms are different in deflagrations and detonations, and, because of this, these are distinct phenomena. Detonations are discussed in Chapter 16.

Principal Characteristics

The temperature profile through a flame is perhaps its most important characteristic. Figure 8.2 illustrates a typical flame temperature profile, together with other essential flame features.

To understand this figure, we need to establish a reference frame for our coordinate system. A flame may be freely propagating, as occurs when a flame is initiated in a tube containing a combustible gas mixture. The appropriate coordinate system would be fixed to the propagating combustion wave. An observer riding with the flame would experience the unburned mixture approaching at the **flame speed, S_L** . This is equivalent to a flat flame stabilized on a burner. Here, the flame is stationary relative to the laboratory reference frame and, once again, the reactants enter the flame with a velocity equal to the flame propagation velocity, S_L . In both examples, we assume that the flame is one dimensional and that the unburned gas enters the flame in a direction normal to the flame sheet. Since a flame creates hot products, the product density is less than the reactant density. Continuity thus requires that the burned gas velocity be greater than the velocity of the unburned gas:

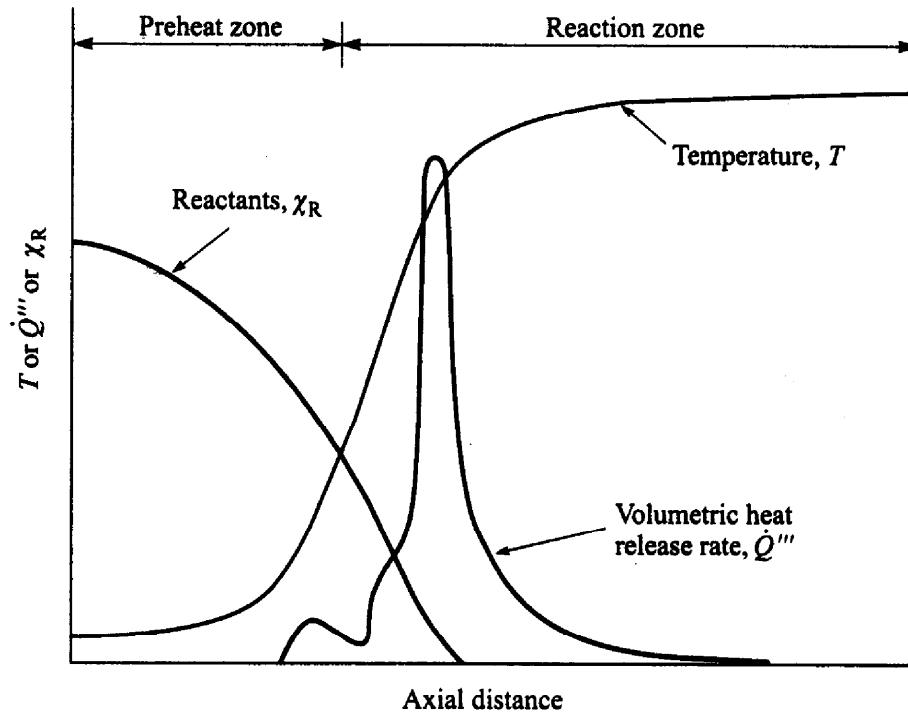


Figure 8.2 Laminar flame structure. Temperature and heat-release-rate profiles based on experiments of Friedman and Burke [1].

$$\rho_u S_L A \equiv \rho_u v_u A = \rho_b v_b A, \quad (8.1)$$

where the subscripts u and b refer to the unburned and burned gases, respectively. For a typical hydrocarbon–air flame at atmospheric pressure, the density ratio is approximately seven. Thus, there is considerable acceleration of the gas flow across the flame.

It is convenient to divide a flame into two zones: the **preheat zone**, where little heat is released; and the **reaction zone**, where the bulk of the chemical energy is released. At atmospheric pressure, the flame thickness is quite thin, on the order of a millimeter. It is useful to divide the reaction zone further into a thin region of very fast chemistry followed by a much wider region of slow chemistry. The destruction of the fuel molecules and the creation of many intermediate species occur in the fast-chemistry region. This region is dominated by bimolecular reactions. At atmospheric pressure, the fast-reaction zone is quite thin, typically less than a millimeter. Because this zone is thin, temperature gradients and species concentration gradients are very large. These gradients provide the driving forces that cause the flame to be self-sustaining: the diffusion of heat and radical species from the reaction zone to the preheat zone. In the secondary reaction zone, the chemistry is dominated by three-body radical recombination reactions, which are much slower than typical bimolecular reactions, and the final burnout of CO via $\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$. This secondary reaction zone may extend several millimeters in a 1-atm flame. Later in this chapter, we present a more detailed description of flame structure illustrating these ideas. Additional information may also be found in Fristrom [2].

Hydrocarbon flames are also characterized by their visible radiation. With an excess of air, the fast-reaction zone appears blue. This blue radiation results from excited CH radicals in the high-temperature zone. When the air is decreased to less than

stoichiometric proportions, the zone appears blue-green, now as a result of radiation from excited C_2 . In both flames, OH radicals also contribute to the visible radiation, and to a lesser degree, chemiluminescence from the reaction $CO + O \rightarrow CO_2 + hv$ [3]. If the flame is made richer still, soot will form, with its consequent blackbody continuum radiation. Although the soot radiation has its maximum intensity in the infrared (recall Wien's law?), the spectral sensitivity of the human eye causes us to see a bright yellow (nearly white) to dull orange emission, depending on the flame temperature. References [4] and [5] provide a wealth of information on radiation from flames.

Typical Laboratory Flames

The Bunsen-burner flame provides an interesting example of laminar premixed flames with which most students have some familiarity and that can be easily used in classroom demonstrations. Figure 8.3a schematically illustrates a Bunsen burner and the flame it produces. A jet of fuel at the base induces a flow of air through the variable area port, and the air and fuel mix as they flow up through the tube. The typical Bunsen-burner flame is a dual flame: a fuel-rich premixed inner flame surrounded by a diffusion flame. The secondary diffusion flame results when the carbon monoxide and hydrogen products from the rich inner flame encounter the ambient air. The shape of the flame is determined by the combined effects of the velocity profile and heat losses to the tube wall. For the flame to remain stationary, the flame speed must equal the speed of the normal component of unburned gas at each location, as illustrated in the vector diagram in Fig. 8.3b. Thus,

$$S_L = v_u \sin \alpha, \quad (8.2)$$

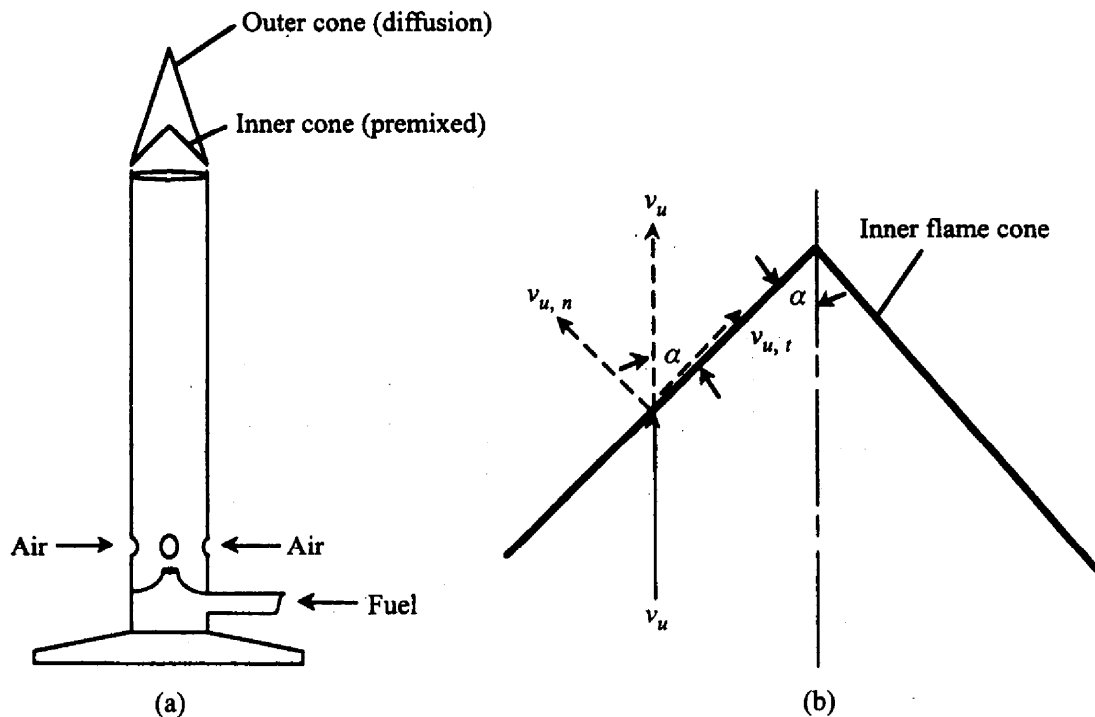


Figure 8.3 (a) Bunsen-burner schematic. (b) Laminar flame speed equals normal component of unburned gas velocity, $v_{u,n}$.

where S_L is the laminar burning velocity. This principle causes the essential conical character of the flame.

One-dimensional flat flames are frequently studied in the laboratory and are also used in some radiant heating burners (Fig. 8.4). Figure 8.5 illustrates the laboratory

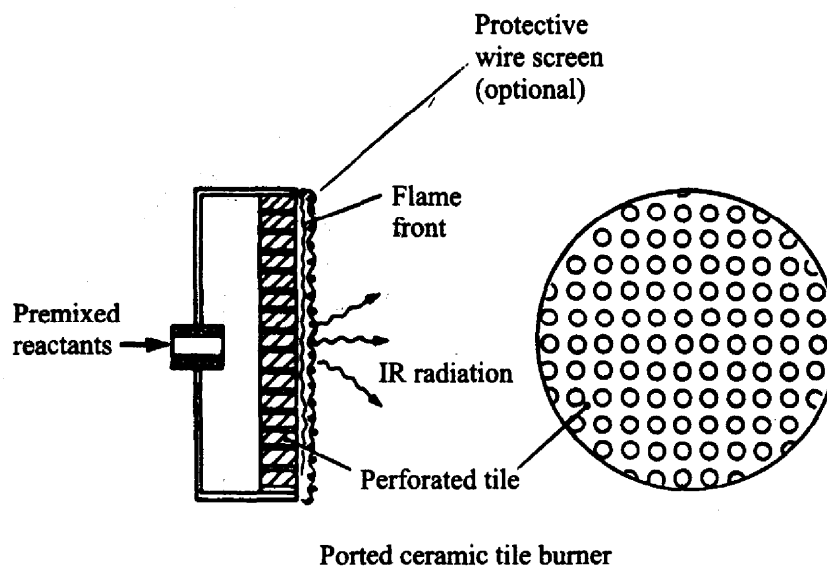
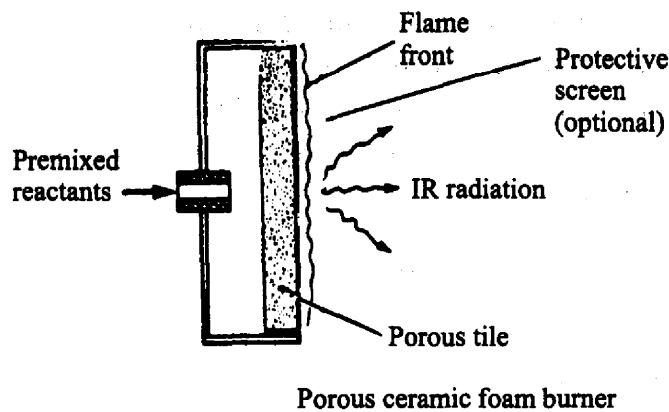
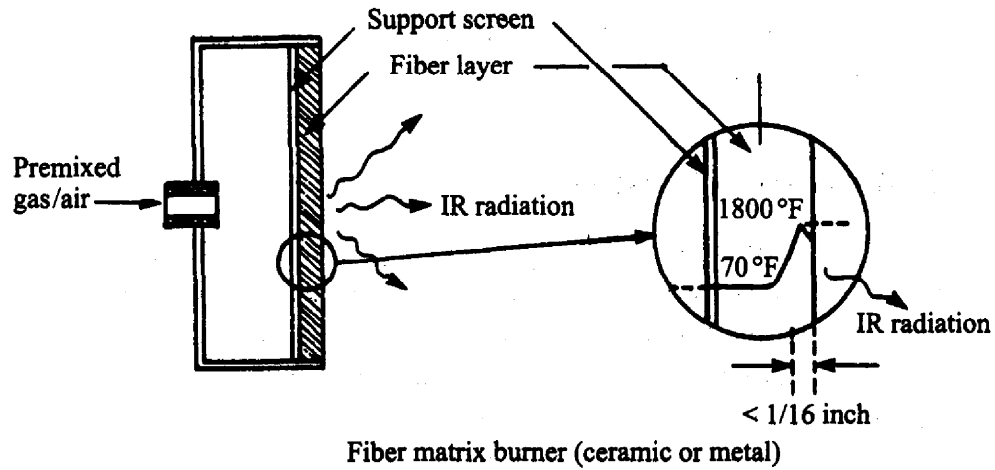


Figure 8.4 Direct-fired radiant burners provide uniform heat flux and high efficiency.
 SOURCE: Reprinted with permission from the Center for Advanced Materials, *Newsletter*, (1), 1990, Penn State University.

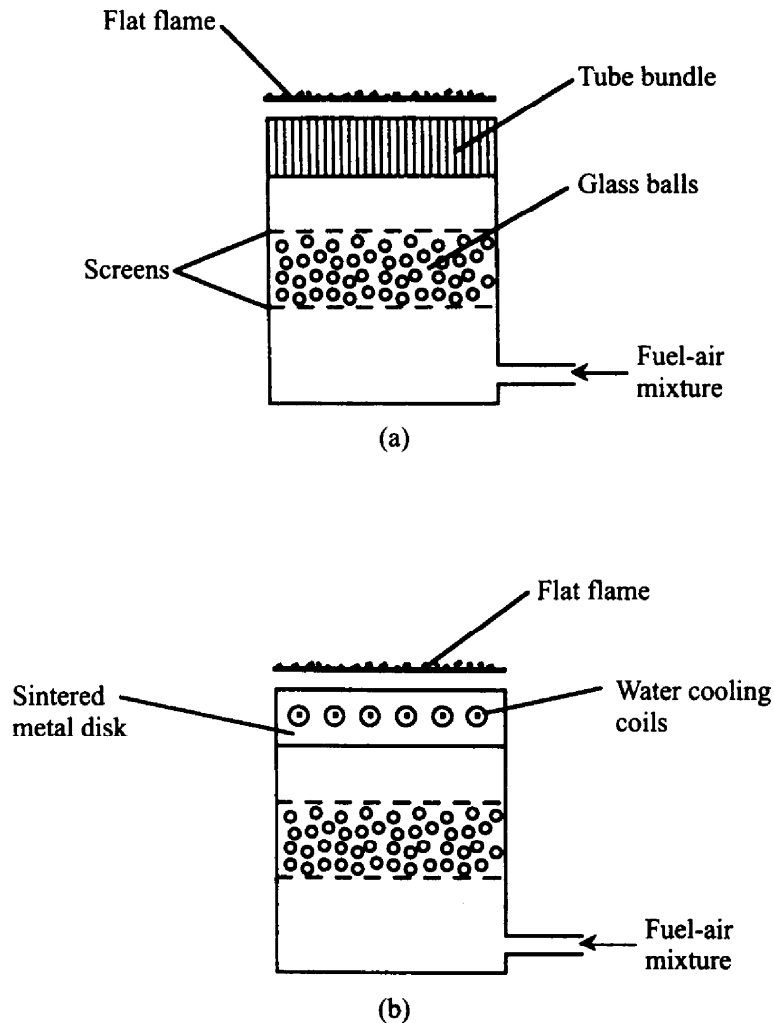


Figure 8.5 (a) Adiabatic flat-flame burner. (b) Nonadiabatic flat-flame burner.

genre. In the adiabatic burner, a flame is stabilized over a bundle of small tubes through which the fuel–air mixture passes lamina­rly [6]. Over a narrow range of conditions, a stable flat flame is produced. The nonadiabatic burner utilizes a water-cooled face that allows heat to be extracted from the flame, which, in turn, decreases the flame speed, allowing flames to be stabilized over a relatively wide range of flow conditions [7].

A premixed laminar flame is stabilized in a one-dimensional gas flow where the vertical velocity of the unburned mixture, v_u , varies linearly with the horizontal coordinate, x , as shown in the lower half of Fig. 8.6. Determine the flame shape and the distribution of the local angle of the flame surface from vertical. Assume the flame speed is independent of position and equal to 0.4 m/s, a nominal value for a stoichiometric methane–air flame.

Example 8.1

Solution

From Fig. 8.7, we see that the local angle, α , which the flame sheet makes with a vertical plane is (Eqn. 8.2),

$$\alpha = \sin^{-1}(S_L / v_u),$$

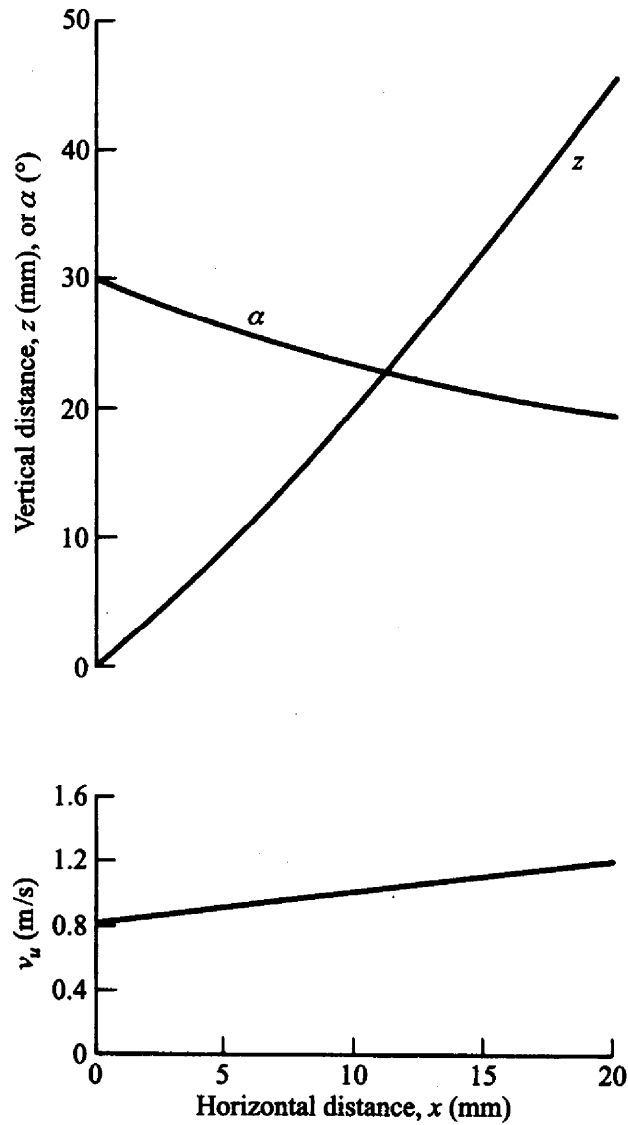


Figure 8.6 Flow velocity, flame position, and angle from vertical of line tangent to flame, for Example 8.1.

where, from Fig. 8.6,

$$v_u \text{ (mm/s)} = 800 + \frac{1200 - 800}{20} x \text{ (mm)}.$$

So,

$$\alpha = \sin^{-1} \left(\frac{400}{800 + 20x \text{ (mm)}} \right),$$

and has values ranging from 30° at $x = 0$ to 19.5° at $x = 20$ mm, as shown in the top part of Fig. 8.6.

To calculate the flame position, we first obtain an expression for the local slope of the flame sheet (dz/dx) in the x - z plane, and then integrate this expression with respect to x to find $z(x)$. From Fig. 8.7, we see that

$$\frac{dz}{dx} = \tan \beta = \left(\frac{v_u^2(x) - S_L^2}{S_L^2} \right)^{1/2},$$

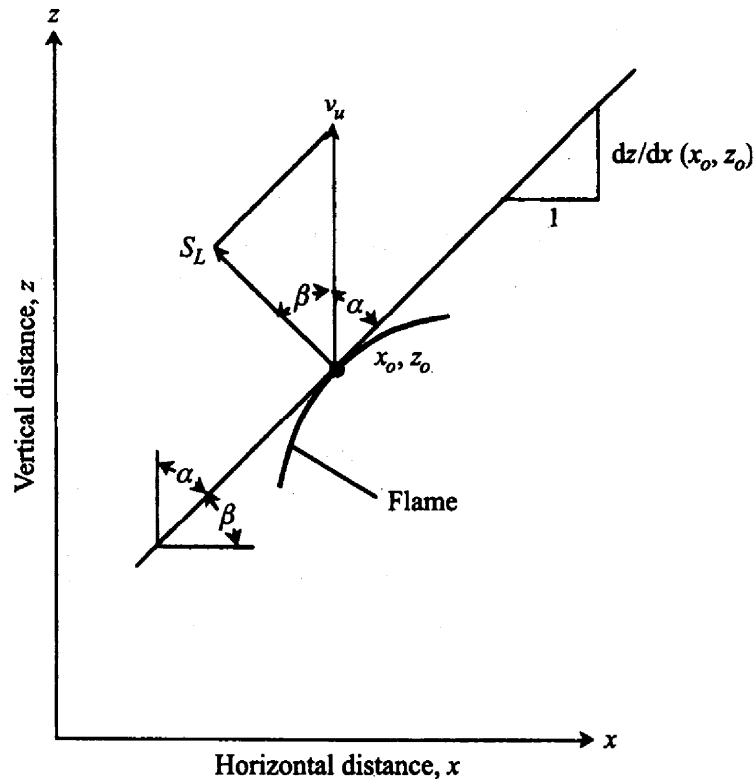


Figure 8.7 Definition of flame geometry for Example 8.1.

which, for $v_u \equiv A + Bx$, becomes

$$\frac{dz}{dx} = \left[\left(\frac{A}{S_L} + \frac{Bx}{S_L} \right)^2 - 1 \right]^{1/2}$$

Integrating the above with $A/S_L = 2$ and $B/S_L = 0.05$ yields

$$\begin{aligned} z(x) &= \int_0^x \left(\frac{dz}{dx} \right) dx \\ &= (x^2 + 80x + 1200)^{1/2} \left(\frac{x}{40} + 1 \right) \\ &\quad - 10 \ln[(x^2 + 80x + 1200)^{1/2} + (x + 40)] \\ &\quad - 20\sqrt{3} + 10 \ln(20\sqrt{3} + 40). \end{aligned}$$

The flame position $z(x)$ is plotted in the upper half of Fig. 8.6. Here we see that the flame sheet is quite steeply inclined. (Note that the horizontal scale is twice that of the vertical.)

Comment

From this example, we see how the flame shape is intimately linked to the velocity distribution of the oncoming unburned gas.

In the next section, we turn our attention to establishing some theoretical basis for how various parameters, such as pressure, temperature, and fuel type, affect laminar flame speeds.

Aviation Gasoline Specifications for aviation gasoline [21] consider combustion characteristics and antiknock quality; fuel metering and aircraft range, as controlled by density and heat of combustion; carburetion and fuel vaporization, controlled by vapor pressure and distillation characteristics; corrosion; fluidity at low temperatures; and fuel cleanliness, handling, and storage stability. The basic composition of aviation gasoline differs from that of automotive gasoline; aviation gasoline consists of alkanes and *iso*-alkanes (50%–60%), cyclanes (20%–30%), small amounts of aromatics (<10%), and essentially no alkenes [9]. This composition contrasts with the somewhat smaller proportions of alkanes, *iso*-alkanes, and cycloalkanes; the presence of alkenes and cycloalkenes; and a greater proportion of aromatics (20%–50%) for automotive gasoline (see Table 17.3). The low aromatic content of aviation fuels results from the combined need to minimize the effects of the fuel on elastomers and to provide a high heating value and proper distillation characteristics [21]. The ASTM standard for aviation gasoline [21] indicates that an aromatics content of more than 25 percent is extremely unlikely. Tetraethyl lead is added to aviation gasoline to meet octane/performance number requirements. The decomposition products of tetraethyl lead scavenge radical species that lead to autoignition.

Aviation Turbine Fuels Specifications for Jet A and Jet A-1 turbine fuels [23] consider a large number of characteristics. Among them are the following: energy content, combustion, volatility, fluidity, corrosion, thermal stability, contaminants, and additives. The heat of combustion (see Chapter 2) is important as it controls the maximum range of an aircraft. The volumetric heating value (MJ/gallon) is the governing parameter for civil aviation [20], and a gravimetric specification (MJ/kg) is given in [23]. Minimizing the production of soot is important to meet emissions requirements and to minimize radiation to the combustor liner (see Chapters 10 and 15). To control soot formation, the aromatics content of the fuel is limited to 25 vol.%, and a minimum smoke point (see Tables 9.5 and 9.6 in Chapter 9) is specified. Aromatics are precursors to soot formation in the combustion of any fuel, and their presence as a fuel component promotes the production of soot. The freezing point is an important property as ambient temperatures at altitude can be quite low. Because the fuel is a mixture of many different hydrocarbons, the various components freeze (become wax) at various temperatures. The ASTM specification [23] of the freezing point is defined as the temperature at which the last wax crystals melt upon heating an initially completely solid fuel. Pumpability is the primary issue associated with fuel freezing, and most fuels will remain pumpable at temperatures slightly below the ASTM freezing point [20]. Jet A-1 fuel owes its existence to having a lower freezing point than Jet A. For more information on aviation fuels, we refer the reader to Refs. [20], [23], and [24].

Natural Gas

Natural gas is typically found within or near oil fields. Natural gas is classified as *associated* or *nonassociated*, depending upon whether it is a product from an oil well (associated gas) or is the product of a gas well (nonassociated). Depending upon its composition, wellhead natural gas, particularly associated gas, must be processed before

Table 17.11 Typical values or ranges of specifications for pipeline-quality natural gas^a

Property or Specification	Typical Value or Range	Comment
Presence of solids	Commercially free	—
Oxygen (O ₂) vol.%	<0.2%–1%	Two companies specified a significantly stricter requirement of <50 ppm.
Carbon dioxide (CO ₂) and nitrogen (N ₂) vol.%	<2% CO ₂ and/or <4% CO ₂ & N ₂ combined	These represent typical specifications from the variety presented in [27]. ^b
Liquid hydrocarbons	No liquid HCs at temperature and pressure of delivery point	—
Hydrogen sulfide (H ₂ S)	5.7–23 mg/m ³	—
Total sulfur	17–460 mg/m ³	In addition to H ₂ S, includes carbonyl sulfide, mercaptans, and mono-, di-, and poly sulfides.
Water (H ₂ O)	65–110 mg/m ³	—
Lower heating value	>36,000 kJ/m ³ typical	34,500 to > 40,900 kJ/m ³ range

^aInformation in this table was compiled from data presented for 18 pipeline companies in Ref. [27]. Values in U.S. customary units have been converted to SI units.

^bCO₂ is removed both to prevent corrosion and to maintain an appropriately high heating value.

Table 17.12 Composition (mol%) and properties of natural gas from sources in the United States [28]^a

Location	CH ₄	C ₂ H ₆	C ₃ H ₈	C ₄ H ₁₀	CO ₂	N ₂	Density ^c (kg/m ³)	HHV ^d (kJ/m ³)	HHV ^d (kJ/kg)
Alaska	99.6	—	—	—	—	0.4	0.686	37,590	54,800
Birmingham, AL	90.0	5.0	—	—	—	5.0	0.735	37,260	50,690
East Ohio ^b	94.1	3.01	0.42	0.28	0.71	1.41	0.723	38,260	52,940
Kansas City, MO	84.1	6.7	—	—	0.8	8.4	0.772	36,140	46,830
Pittsburgh, PA	83.4	15.8	—	—	—	0.8	0.772	41,840	54,215

^aAlthough not explicitly stated in Ref. [28], these gases appear to be pipeline gases.

^bAlso contains 0.01% H₂ and 0.01% O₂.

^cAt 1 atm and 15.6°C (60 F).

^dHigher heating values for 1 atm and 15.6°C (60 F) [28].

Table 17.13 Composition (mol%) and properties of natural gas from worldwide sources [28]^a

Location	CH ₄	C ₂ H ₆	C ₃ H ₈	C ₄ H ₁₀	CO ₂	N ₂	Density ^b (kg/m ³)	HHV ^c (kJ/m ³)	HHV ^c (kJ/kg)
Algeria LNG	87.2	8.61	2.74	1.07	—	0.36	0.784	42,440	54,130
Groningen, Netherlands	81.2	2.9	0.36	0.14	0.87	14.4	0.784	33,050	42,150
Kuwait, Bergen	86.7	8.5	1.7	0.7	1.8	0.6	0.784	40,760	51,990
Libya LNG	70.0	15.0	10.0	3.5	—	0.90	0.956	49,890	52,210
North Sea, Bacton	93.63	3.25	0.69	0.27	0.13	1.78	0.723	38,450	53,200

^aAlthough not explicitly stated in Ref. [28], these gases appear to be pipeline gases.

^bAt 1 atm and 15.6°C (60 F).

^cHigher heating values for 1 atm and 15.6°C (60 F) [28].

it can enter distribution pipeline systems. Unprocessed natural gas is primarily methane, with smaller quantities of other light (C₂–C₈) hydrocarbons. Noncombustible gases, N₂, CO₂, and He, are also frequently present. Hydrogen sulfide, mercaptans, water, oxygen, and other trace contaminants may be present. Separation of dissolved associated gas from crude oil is frequently not economical [9]; nevertheless, the amount of gas flared or vented annually worldwide is huge—110 billion cubic meters, the equivalent to the combined annual natural gas consumption of France and Germany [25]. However, initiatives are in place to significantly reduce flaring of associated gas [25].

Although there are no industry or governmental standards for pipeline natural gas, contracts between producers and pipeline companies define general ranges of composition and other properties [26, 27]. Processing removes solid matter (e.g., sand), liquid hydrocarbons, sulfur compounds, water, nitrogen, carbon dioxide, helium, and any other undesirable compounds to meet contract specifications. The removal of sulfur compounds results in making an acidic, i.e., *sour*, gas *sweet*. Table 17.11 shows typical values, or ranges, of important properties of pipeline gas based on the *General Terms and Conditions* of a set of geographically dispersed pipeline companies in the United States and Canada.

The composition of natural gas varies widely depending upon the source. Examples for U.S. sources of natural gas are shown in Table 17.12. Compositions for natural gases from a variety of non-U.S. sources are provided in Table 17.13.

Using the 298.15 K reference state, calculate the higher heating value (HHV) for the natural gas from the Bergen field in Kuwait shown in Table 17.13. Compare the result with the value given in Table 17.13.

Example 17.2

Solution

Our solution follows that of Example 2.4. From Fig. 2.9, we see that the HHV can be expressed as

$$\text{HHV} = \Delta h_c = (H_{\text{reac}} - H_{\text{prod}}) / MW_{\text{fuel}} \text{ (kJ/kg}_{\text{fuel}}\text{)}$$

where

$$H_{\text{reac}} = \sum_{\text{Reac}} N_i \bar{h}_{f,i}^{\circ} \quad \text{and} \quad H_{\text{prod}} = \sum_{\text{Prod}} N_i \bar{h}_{f,i}^{\circ}$$

Using the given composition of the natural gas, we can calculate the apparent molecular weight of the fuel (natural gas) as

$$MW_{\text{fuel}} = \sum \chi_i MW_i = \chi_{\text{CH}_4} MW_{\text{CH}_4} + \chi_{\text{C}_2\text{H}_6} MW_{\text{C}_2\text{H}_6} + \chi_{\text{C}_3\text{H}_8} MW_{\text{C}_3\text{H}_8} + \chi_{\text{CO}_2} MW_{\text{CO}_2} + \chi_{\text{N}_2} MW_{\text{N}_2}$$

Substituting numerical values, we obtain

$$\begin{aligned} MW_{\text{fuel}} &= 0.867(16.043) + 0.085(30.069) + 0.017(44.096) + 0.018(44.011) + 0.006(28.013) \\ &= 18.175 \text{ kg/kmol}_{\text{fuel}} \end{aligned}$$

The reactant enthalpy H_{reac} is evaluated using the given fuel composition and the enthalpies-of-formation: