表 1.1: H_2-O_2 反応機構 (Chemkin 形式)

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reactions
! - major three chain branching/propagation reactions
 H+O2=OH+O                   9.756e+013   0.000   14844.6
 O+H2=OH+H                   5.120e+004   2.670    6278.7
 H2O+H=H2+OH                 4.520e+008   1.600   18422.6
! - major near-termination forming HO2
 H+O2+M=HO2+M                2.100e+018  -0.800       0.0
          N2/0.67/ O2/0.4/ CO2/1.5/ H2O/0/ AR/0.29/
 O2+H+H2O=HO2+H2O            6.890e+015   0.000   -2086.5
! - OH/HO2 radical chain degradation/termination
 OH+OH=O+H2O                 1.510e+009   1.140     100.4
 OH+HO2=H2O+O2               2.890e+013   0.000    -497.1
 H+HO2=H2+O2                 4.280e+013   0.000    1410.1
 HO2+HO2=H2O2+O2             4.220e+014   0.000   11983.7
          duplicate
 HO2+HO2=H2O2+O2             1.320e+011   0.000   -1630.0
          duplicate
! - HO2 radical chain reactivation/propagation
 H+HO2=OH+OH                 1.690e+014   0.000     874.8
 H+HO2=H2O+O                 3.010e+013   0.000    1720.8
 O+HO2=O2+OH                 3.190e+013   0.000       0.0
! - H2O2 reactions
 OH+OH(+M)=H2O2(+M)          7.230e+013  -0.370       0.0
                       low / 5.530e+019  -0.760       0.0 /
          troe / 1 1 1 1040 /
          N2/0.4/ O2/0.4/ CO2/1.5/ H2O/6.5/ AR/0.35/
 H2O2+H=HO2+H2               1.690e+012   0.000    3754.8
 H2O2+H=OH+H2O               1.020e+013   0.000    3577.9
 H2O2+O=OH+HO2               6.620e+011   0.000    3974.7
 H2O2+OH=H2O+HO2             7.830e+012   0.000    1331.3
! - recombination chain termination/degradation
 H+H+M=H2+M                  1.870e+018  -1.000       0.0
          N2/0.4/ O2/0.4/ CO2/1.5/ H2O/6.5/ AR/0.35/
 H+H+H2=H2+H2                9.790e+016  -0.600       0.0
 H+O+M=OH+M                  1.180e+019  -1.000       0.0
          N2/0.4/ O2/0.4/ CO2/1.5/ H2O/6.5/ AR/0.35/
 H+OH+M=H2O+M                5.530e+022  -2.000       0.0
          N2/0.4/ O2/0.4/ CO2/1.5/ H2O/2.55/ AR/0.15/
 O+O+M=O2+M                  5.400e+013   0.000   -1787.8
          N2/0.4/ O2/0.4/ CO2/1.5/ H2O/6.5/ AR/0.35/
end
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表 1.2: Cl_2-H_2 連鎖反応系の反応速度定数

反応	A [cm^3 mol^{-1} s^{-1}]	E_a / R [K]	k (298 K) [cm^3 mol^{-1} s^{-1}]
(1) $Cl + H_2 \rightarrow H + HCl$	2.2×10^{13}	2300	9.8×10^{9}
(2) $H + Cl_2 \rightarrow Cl + HCl$	4.8×10^{13}	416	1.2×10^{13}

表 1.3: H_2-O_2 連鎖反応系の反応速度定数

反応	A [cm^3 mol^{-1} s^{-1}]	b	E_a / R [K]	k (1000 K) [cm^3 mol^{-1} s^{-1}]
(1) $H + O_2 \rightarrow OH + O$	9.8×10^{13}	0	7470	5.6×10^{10}
(2) $O + H_2 \rightarrow OH + H$	5.1×10^{4}	2.67	3160	2.2×10^{11}
(3) $OH + H_2 \rightarrow H_2O + H$	1.0×10^{8}	1.6	1660	1.2×10^{12}
*(4) $H + O_2 + M \rightarrow HO_2 + M$	1.7×10^{18}	–0.8	0	6.8×10^{15}
(11) $H + HO_2 \rightarrow OH+OH$	1.7×10^{14}	0.0	440	1.1×10^{14}

*(4) のみ A と k (1000K) の単位: cm^6 mol^{-2} s^{-1}

$[H_2]$:$[O_2]$ = 2:1, p = 0.01 atm, T = 1000 K で

$[H_2] = 8.12 \times 10^{-8}$, $[O_2] = 4.06 \times 10^{-8}$, $[M] = [H_2] + [O_2] = 1.22 \times 10^{-7}$ (mol cm^{-3})

$r_1 = k_1[O_2] = 2.3 \times 10^{3}$ s^{-1}

$r_2 = k_2[H_2] = 1.8 \times 10^{4}$ s^{-1}

$r_3 = k_3[H_2] = 9.7 \times 10^{4}$ s^{-1}

$r_4 = k_4[O_2][M] = 3.4 \times 10^{1}$ s^{-1}

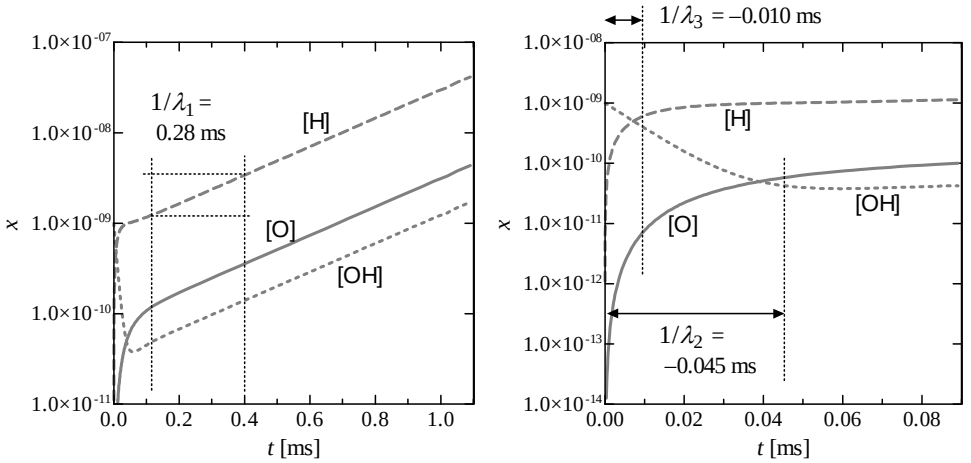

図 1.1: H_2-O_2 連鎖反応

[H_2:O_2 = 2:1, p = 0.01 atm, T = 1000 K, $x(OH)_0 = 1 \times 10^{-9}$]