

表 1.1: H₂-O₂ 反応機構 (Chemkin 形式)

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 H2O2				
H+O2+M=H2O2+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=H2O2+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	
H2O+HO2=H2O2+O2	4.220e+014	0.000	11983.7	
duplicate				
H2O+HO2=H2O2+O2	1.320e+011	0.000	-1630.0	
duplicate				
! - H2O2 radical chain reactivation/propagation				
H+H2O2=OH+OH	1.690e+014	0.000	874.8	
H+H2O2=H2O+O	3.010e+013	0.000	1720.8	
O+H2O2=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				

表 1.2: Cl₂-H₂ 連鎖反応系の反応速度定数

反応	A [m ³ mol ⁻¹ s ⁻¹]	E _a / R [K]	k (298 K) [m ³ mol ⁻¹ s ⁻¹]
(1) Cl + H ₂ → H + HCl	2.2 × 10 ⁷	2300	9.8 × 10 ³
(2) H + Cl ₂ → Cl + HCl	4.8 × 10 ⁷	416	1.2 × 10 ⁷

表 1.3: H₂-O₂ 連鎖反応系の反応速度定数

反応	A [m ³ mol ⁻¹ s ⁻¹]	b	E _a / R [K]	k (1000 K) [m ³ mol ⁻¹ s ⁻¹]
(1) H + O ₂ → OH + O	9.8 × 10 ⁷	0	7470	5.6 × 10 ⁴
(2) O + H ₂ → OH + H	5.1 × 10 ⁻²	2.67	3160	2.2 × 10 ⁵
(3) OH + H ₂ → H ₂ O + H	1.0 × 10 ²	1.6	1660	1.2 × 10 ⁶
* (4) H + O ₂ + M → HO ₂ + M	1.7 × 10 ⁶	-0.8	0	6.8 × 10 ³

* (4) のみ A と k (1000K) の単位: m⁶ mol⁻² s⁻¹

[H₂]:[O₂] = 2:1, p = 1013.25 Pa (0.01 atm), T = 1000 K で

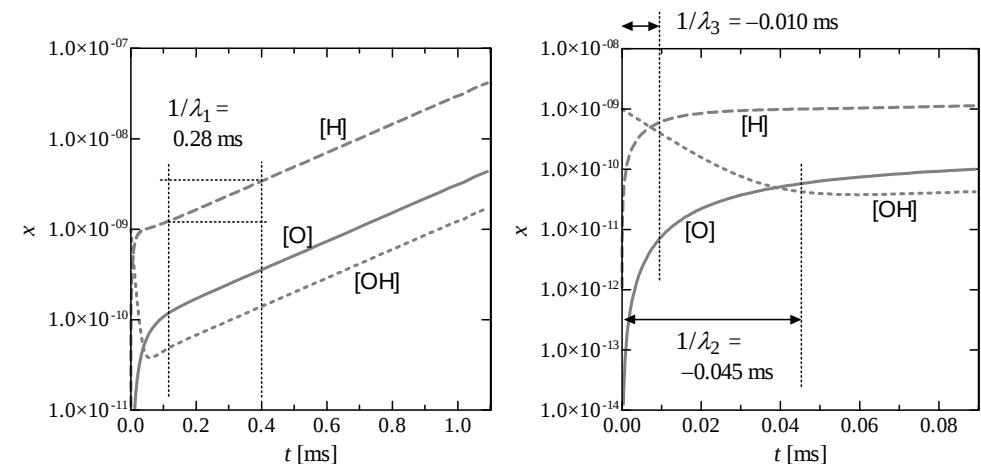
[H₂] = 8.12 × 10⁻², [O₂] = 4.06 × 10⁻², [M] = [H₂] + [O₂] = 1.22 × 10⁻¹ (mol m⁻³)

r₁ = k₁[O₂] = 2.3 × 10³ s⁻¹

r₂ = k₂[H₂] = 1.8 × 10⁴ s⁻¹

r₃ = k₃[H₂] = 9.7 × 10⁴ s⁻¹

r₄ = k₄[O₂][M] = 3.4 × 10¹ s⁻¹

図 1.1: H₂-O₂ 連鎖反応

[H₂:O₂ = 2:1, p = 1013.25 Pa (0.01 atm), T = 1000 K, x(OH)₀ = 1 × 10⁻⁹]