

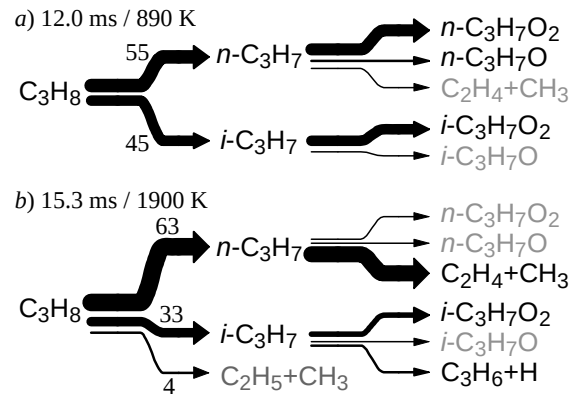


図 2.1: 反応経路解析の例

プロパン-空気当量混合気の定容断熱計算
 (40 atm, 850 K) における燃料消費過程の
 経路解析. a) 着火誘導期, b) 熱炎領域

表 2.1 H₂-O₂ 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 → OH + O	9.8 × 10 ¹³	0	7470	5.6 × 10 ¹⁰
(2) O + H ₂ → OH + H	5.1 × 10 ⁴	2.67	3160	2.2 × 10 ¹¹
(3) OH + H ₂ → H ₂ O + H	1.0 × 10 ⁸	1.6	1660	1.2 × 10 ¹²
*(4) H + O ₂ + M → HO ₂ + M	1.7 × 10 ¹⁸	-0.8	0	6.8 × 10 ¹⁵
(11) H + HO ₂ → OH + OH	1.7 × 10 ¹⁴	0.0	440	1.1 × 10 ¹⁴

* A と k (1000K) の単位: cm⁶ mol⁻² s⁻¹

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

[H₂] = 8.12 × 10⁻⁸, [O₂] = 4.06 × 10⁻⁸, {M} = [H₂] + [O₂] = 1.22 × 10⁻⁷ (mol cm⁻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

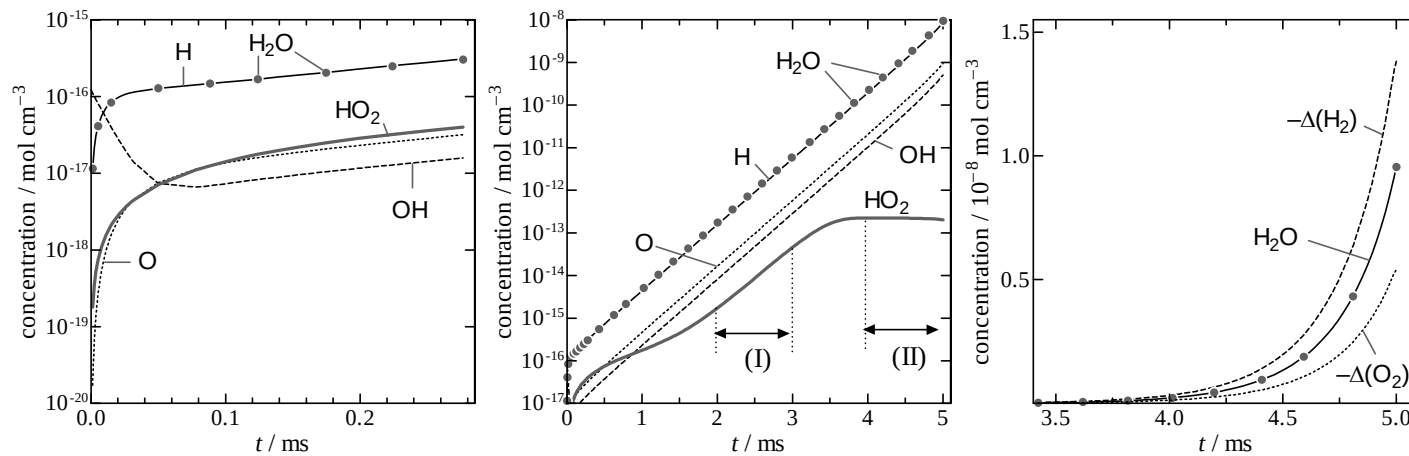
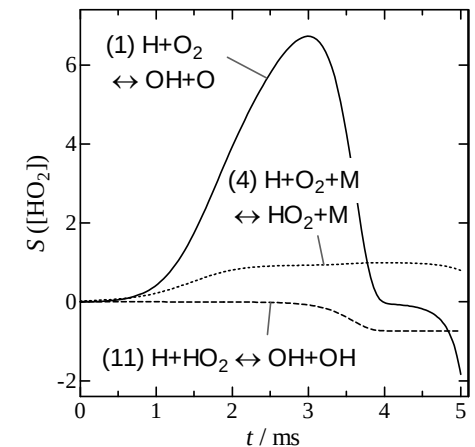
r₄ = k₄[O₂][M] = 3.4 × 10¹ s⁻¹

表 2.2: senkin 入力の例

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SENS
CONV
PRES 0.01
TEMP 1000.
TIME 5.E-3
DELT 2.E-4
REAC H2 2.
REAC O2 1.
REAC OH 3.E-9
END

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図 2.2: H₂-O₂ 連鎖反応 ([H₂]:[O₂] = 2:1, p = 0.01 atm, T = 1000 K, x[OH]₀ = 1 × 10⁻⁹)図 2.3: HO₂ 濃度に対する感度係数
(計算条件: 図 2.2 と同じ)