Ignition of hydrogen-air mixtures under volumetric expansion

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outlines

Formation of expansion waves

SW-obstacle

SW diffraction

Expansions can be formed in complex pipelines

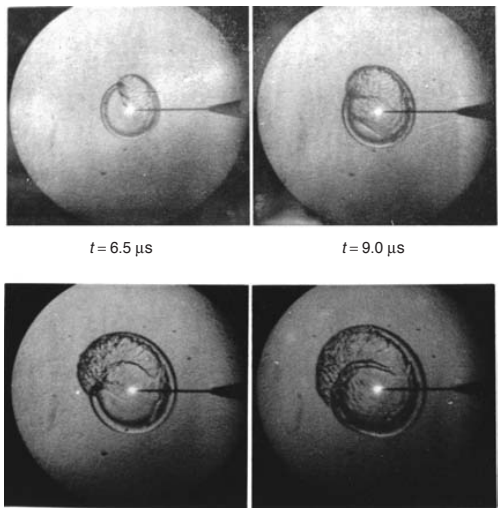
Important for shock ignition and industrial safety

Simulations by Prof. H. Hornung

Re-initiation behind a decaying shock wave (1)

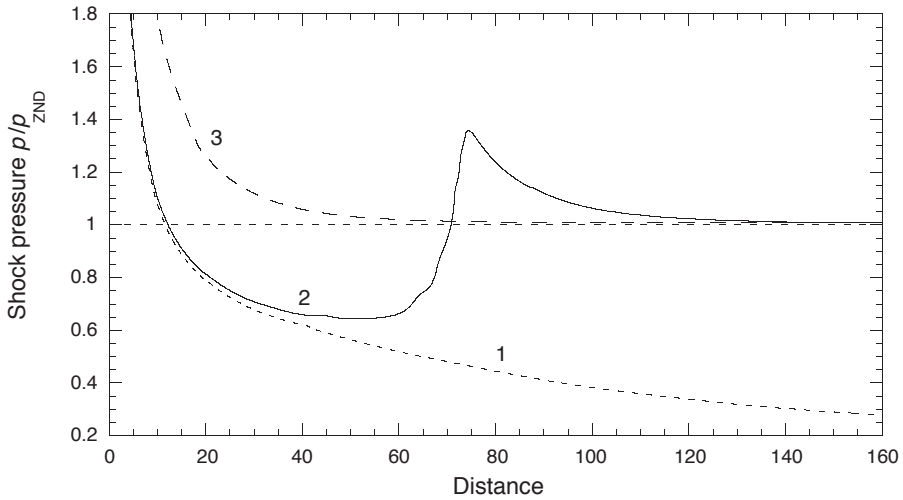
Detonation direct initiation

2-D images



Bach et al., 1969

1-D simulations



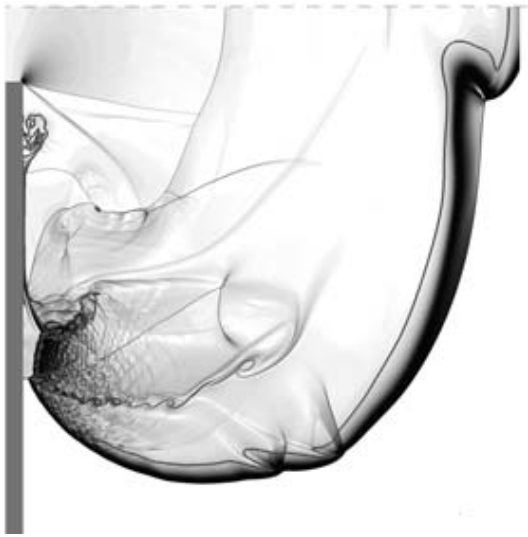
Ng and Lee, 2003

SW velocity decreases much below D_{CJ} before re-initiation occurs

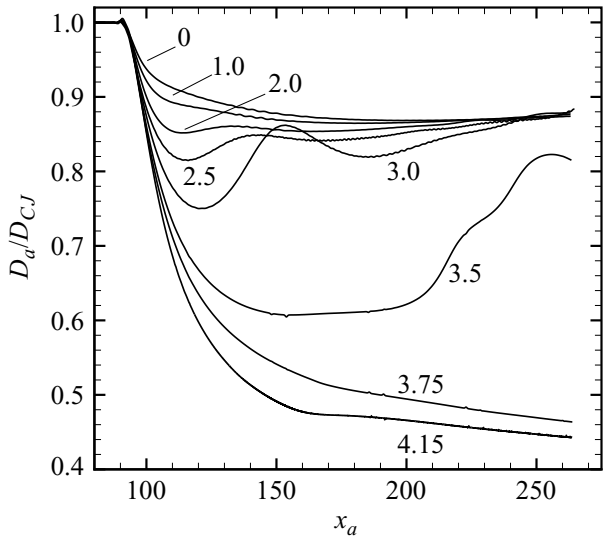
Re-initiation behind a decaying shock wave (2)

Detonation diffraction

2-D simulations



Velocity along the axis



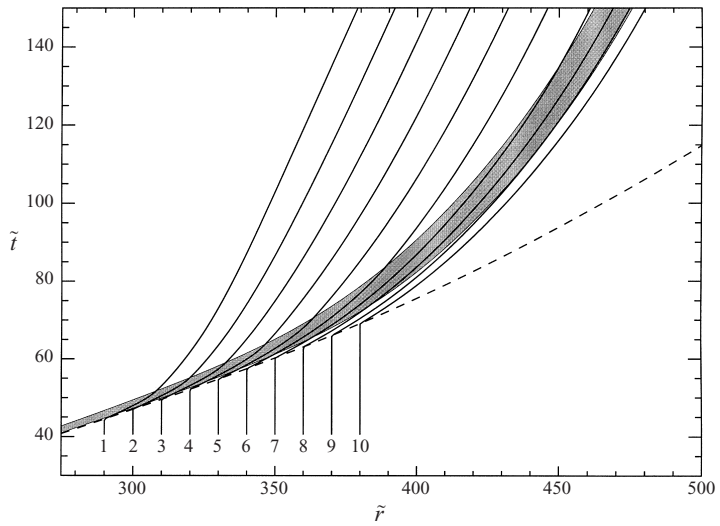
SW velocity decreases much below D_{CJ} before re-initiation occurs

Results from Arienti and Shepherd, 2005

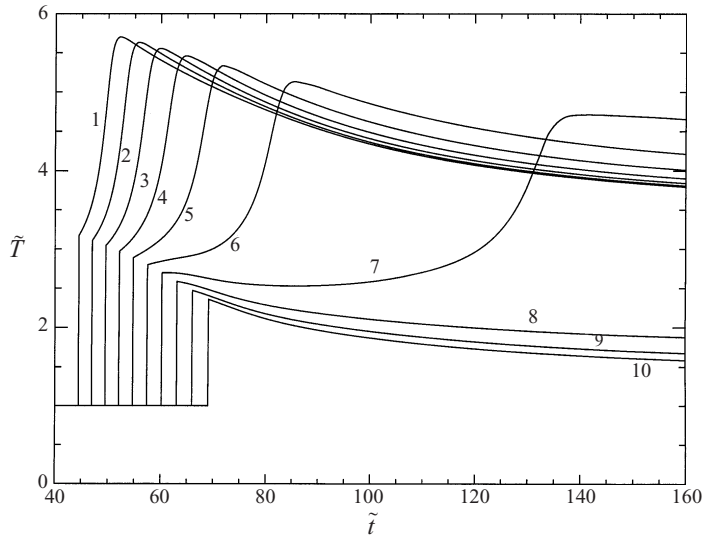
Reaction in expanding flows (1)

Lagrangian particles

Particle path



Temperature profile



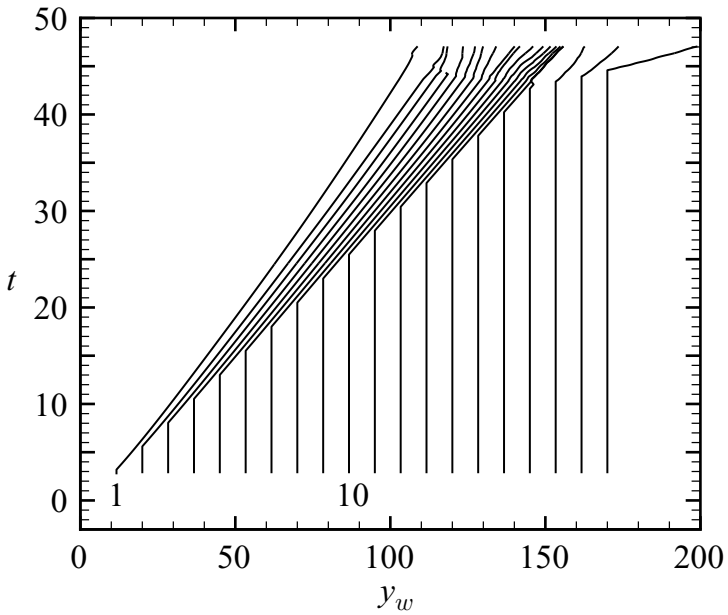
As the SW decays, ignition delay-time increases and the reaction is eventually quenched

Results from Eckett et al., 2000

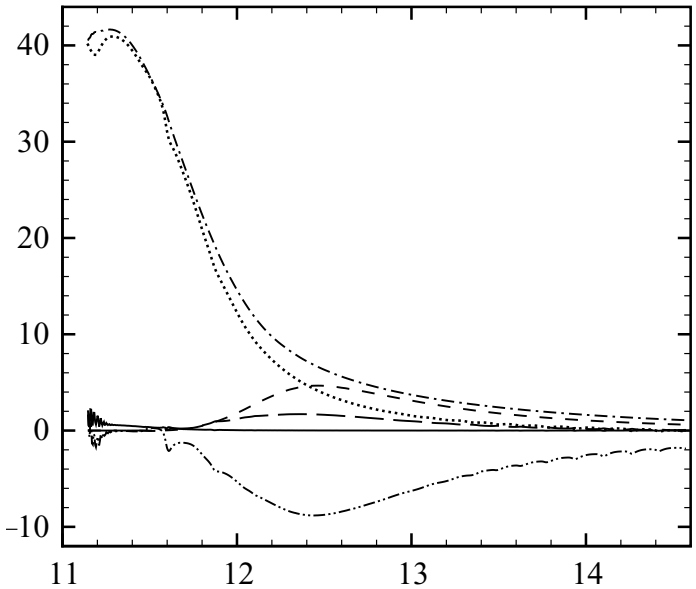
Reaction in expanding flows (2)

Ignition dynamics

Particle path



Energy equation analysis

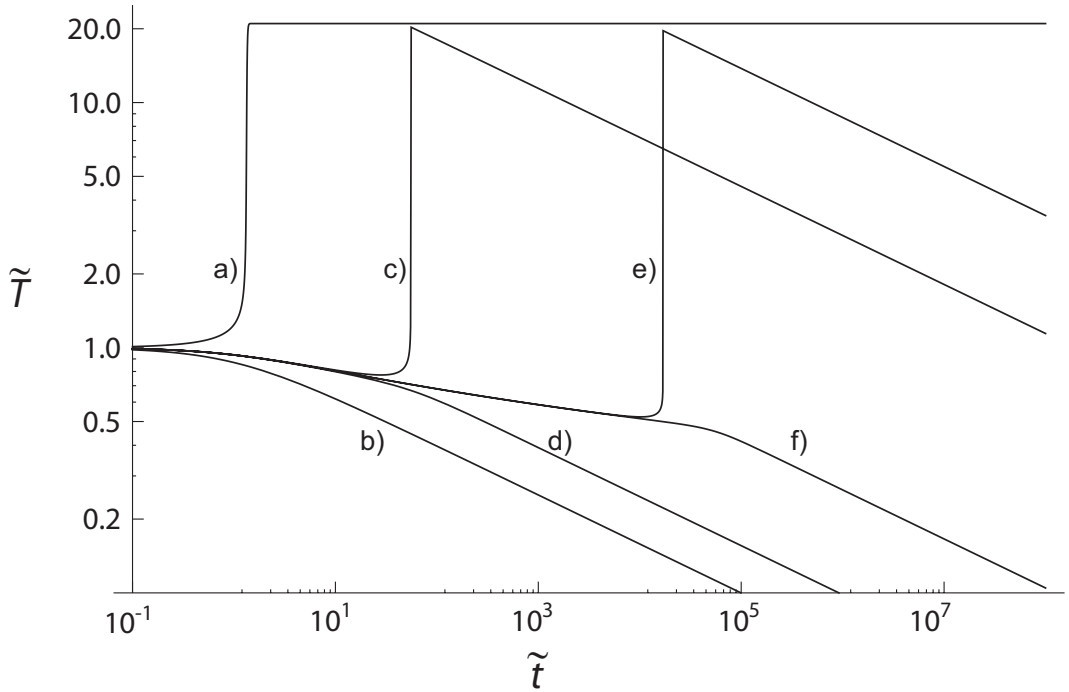


Chemical energy release vs unsteadiness

Results from Arienti and Shepherd, 2005

Previous work on reacting expanding flows

Lundstrom and Oppenheim, Eckett et al., Arienti and Shepherd, Radulescu and Maxwell



1-step chemical models were used

Purpose of the study

Investigate the effect of volumetric expansion on the chemical kinetics of hydrogen-air mixtures

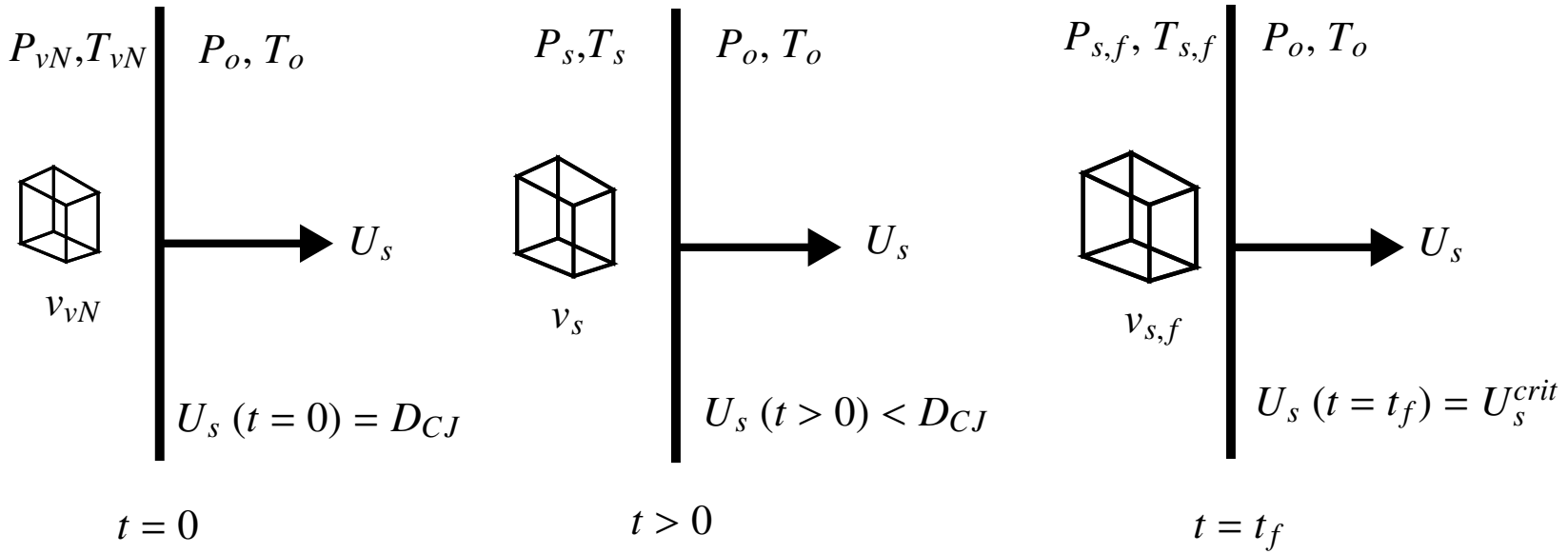
Approach

- **Chemistry : detailed reaction model**
- **Flow : simple reactor model to describe expansion**
- **Scope : perform detailed kinetics analyses**

outlines

Problem definition

Specific volume behind a decaying SW



Gas expands behind SW as time progresses

Chemical reactions do not take place at constant pressure or volume...
cooling needs to be considered

Mathematical formulation (1)

Three forms for the rate of SW velocity decrease

- **Linear :** $U_S(t) = D_{CJ} - \alpha t$
- **Exponential :** $U_S(t) = D_{CJ} \exp(-\beta t)$
- **Power law :** $U_S(t^*) = D_{CJ} (t^*)^{-\delta}$

α, β, and δ are adjusted so that $\Delta T / \tau$ through isentropic expansion is the same

- **Linear :** $\alpha(\Delta T) = D_{CJ} - U_S(\Delta T)$
- **Exponential :** $\beta(\Delta T) = \ln(D_{CJ}/U_S(\Delta T))$
- **Power law :** $\delta(\Delta T) = \frac{\ln(D_{CJ}/U_S(\Delta T))}{\ln(2)}$

Mathematical formulation (2)

Final time of simulation

- **Linear :** $t_{f,Lin} = \frac{D_{CJ} - U_S^{crit}}{\alpha(\Delta T)}$
- **Exponential :** $t_{f,Exp} = \frac{\ln(D_{CJ}/U_S^{crit})}{\beta(\Delta T)}$
- **Power law :** $t^*_{f,Pw} = \left(\frac{D_{CJ}}{U_S^{crit}}\right)^{1/\delta(\Delta T)}$

When SW becomes an acoustic wave ($M \sim 1$)

Calculation procedure

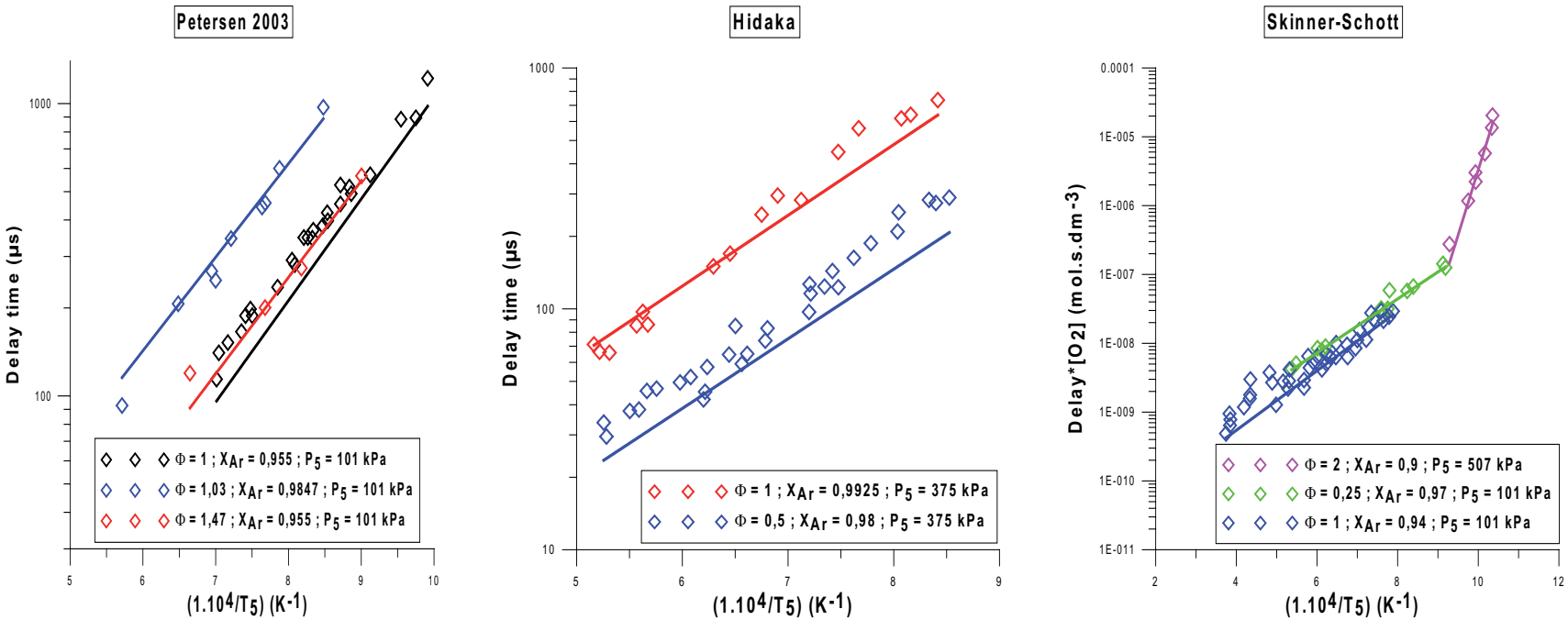
Numerical routine including the following steps

- Calculate D_{CJ}
- Calculate P_{vN} and T_{vN} for $U_S = D_{CJ}$
- Calculate τ_{Th} at P_{vN} and T_{vN} using a CP reactor
- Calculate $P_S(\Delta T)$ using the isentropic relationship for a given ΔT
- Calculate the corresponding $U_S(\Delta T)$
- Calculate the shock decay rates coefficients : α, β and δ
- Calculate t_f (or t_f^*) for all decay rates
- Construct time vector in the range [0, t_f]
- Calculate shock velocity, U_S, corresponding to each element of the time vector
- Calculate $P_S(t)$ corresponding to each value of $U_S(t)$
- Calculate specific volume, v, starting from P_{vN} and T_{vN}, and considering an isentropic expansion
- Calculate τ_{Th} with the volume vs. time option (VTIM)

outlines

Reaction model validation (1)

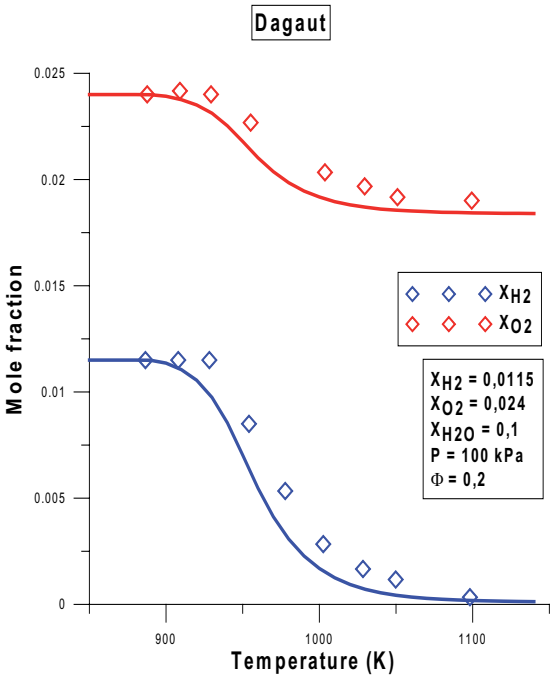
Shock tube data

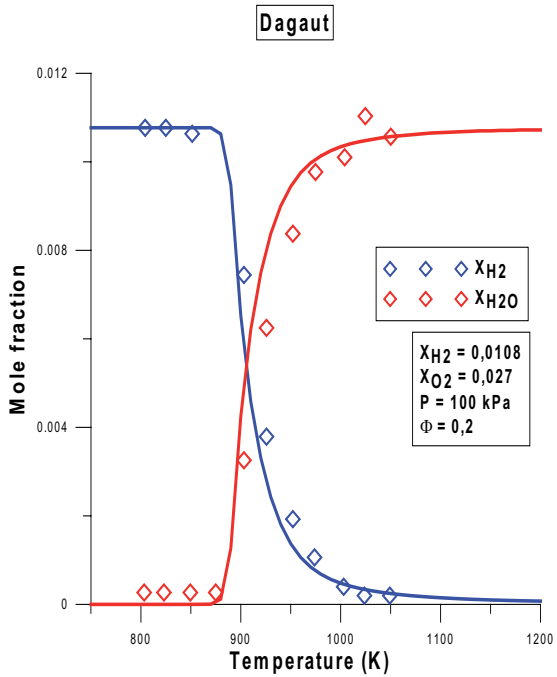


Good agreement

Reaction model validation (2)

Jet-stirred reactor data

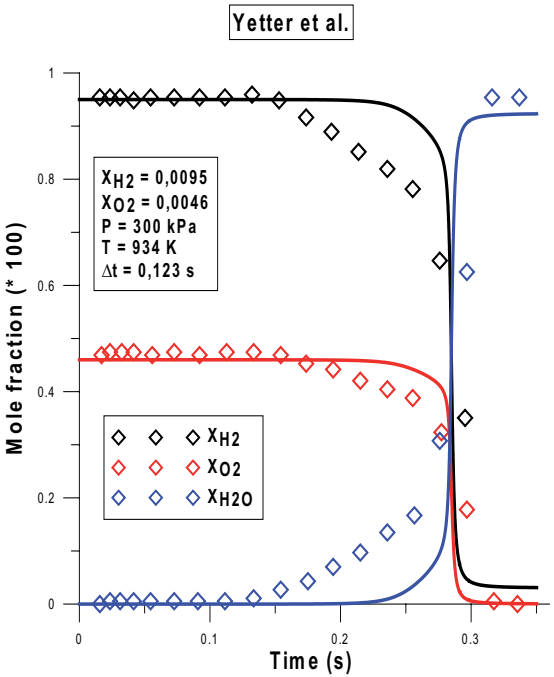


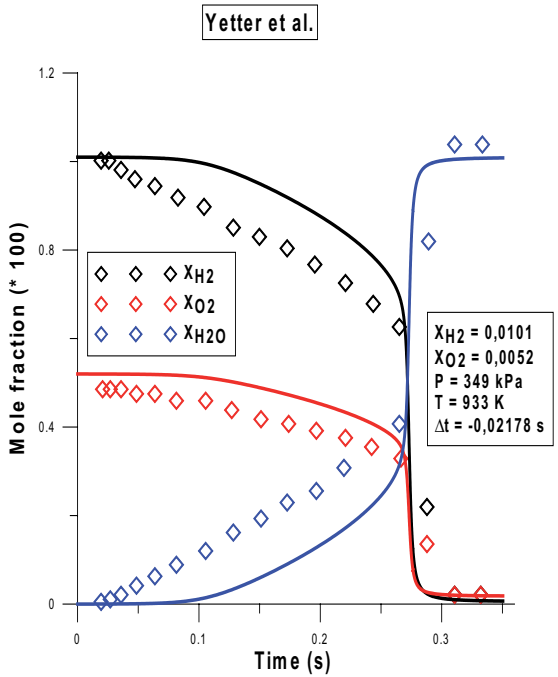


Good agreement

Reaction model validation (3)

Flow reactor data



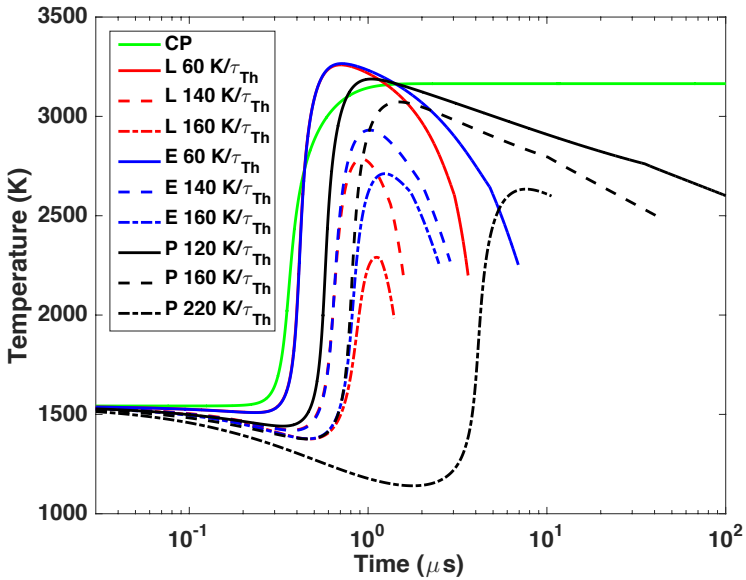


Reasonable agreement

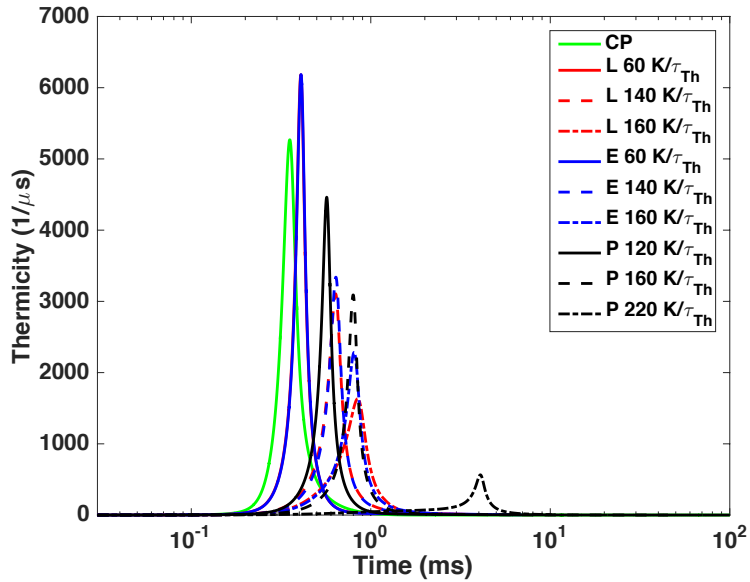
Effect of expansion on the ignition dynamics

Cooling rate 0-250 K/τ

Temperature profiles



Thermicity profiles



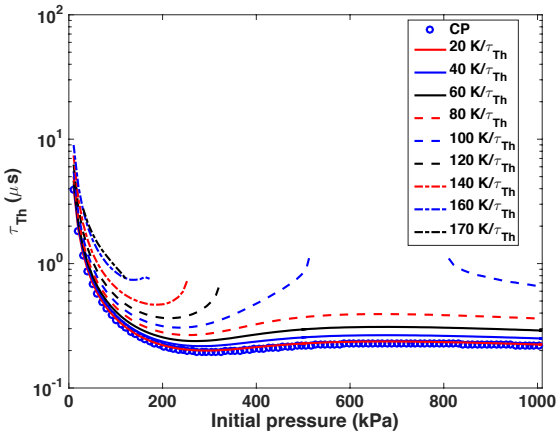
As cooling rate is increased

τ increases and σ_{max} decreases

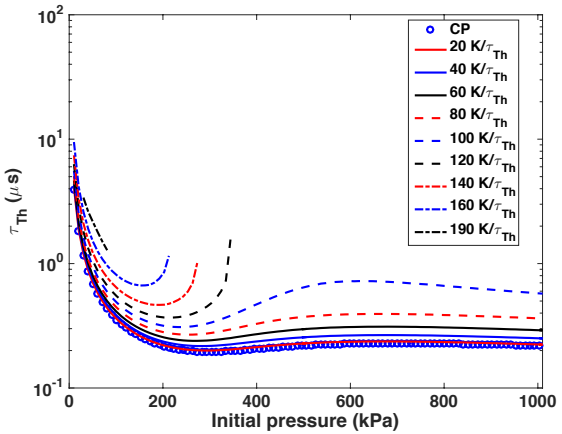
Effect of expansion on τ

P_1 = 10-1000 kPa and Cooling rate 0-250 K/τ

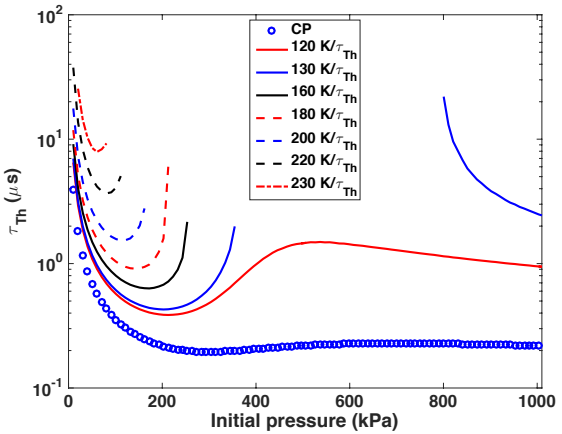
Linear decay



Exponential decay



Power law decay



Highest sensitivity to quenching for P_1 = 500-800 kPa

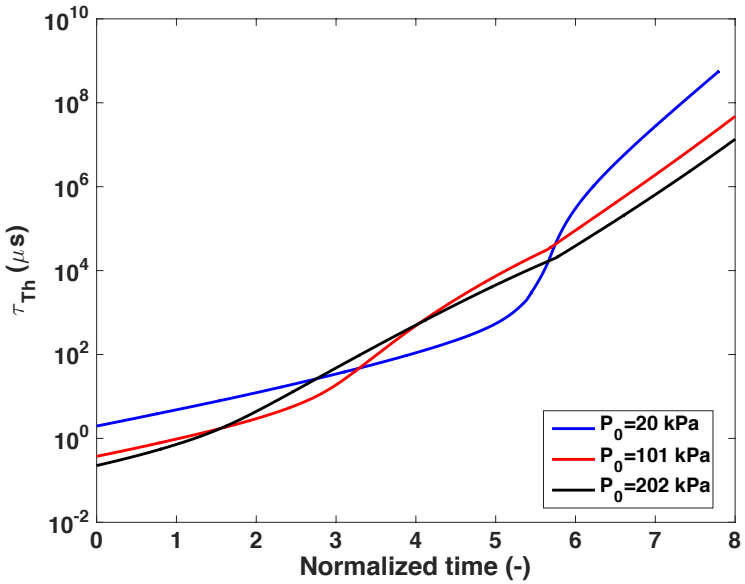
Lowest sensitivity to quenching for P_1 < 100 kPa

Variation of CP τ along isentropes

Effect of initial pressure

Low pressure range

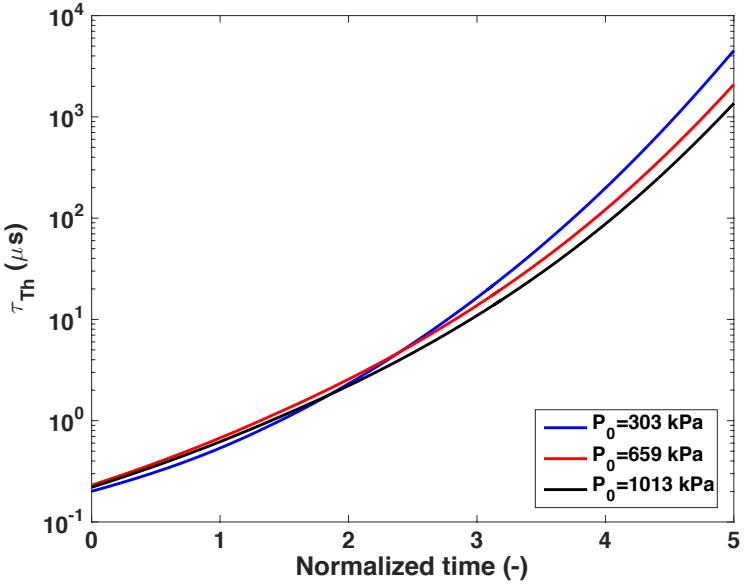
(Exponential decay)



140 K/τ_{Th}

High pressure range

(Linear decay)



100 K/τ_{Th}

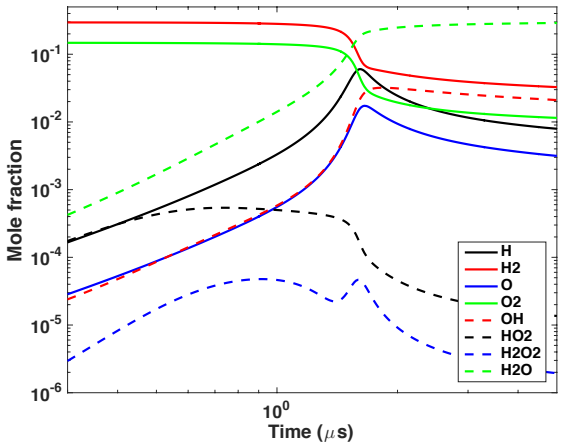
At LP, 2nd explosion limit is located at lower T

At HP, delay-time decreases as P increases

Species profiles

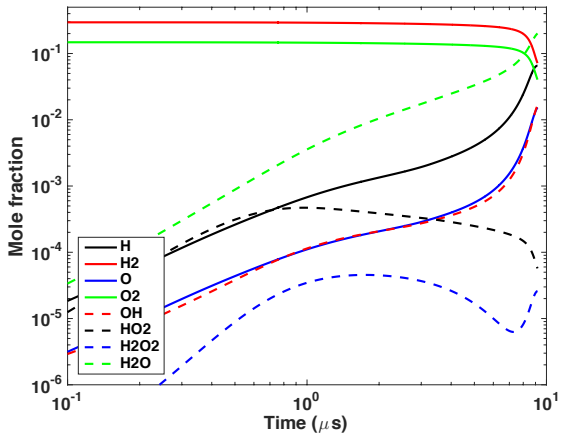
Power law decay rate

Sub-critical



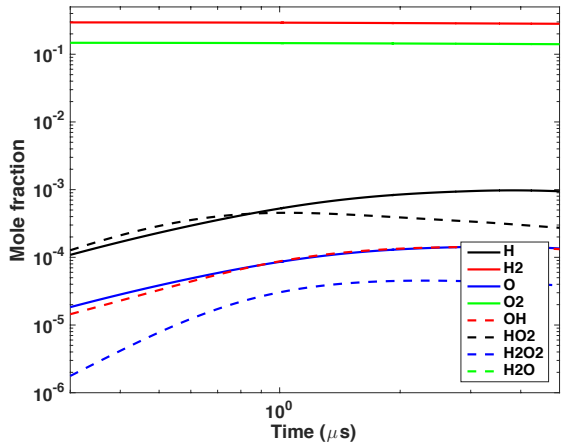
200 K/τ

Near-critical



225 K/τ

Super-critical



230 K/τ

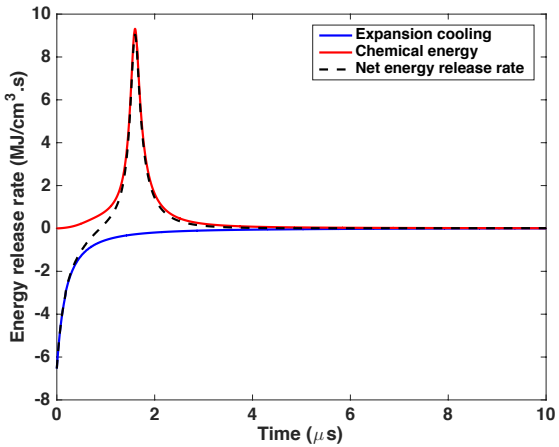
At 225 K/τ, runaway just before final time

At 230 K/τ, no significant consumption of reactants

Energy release

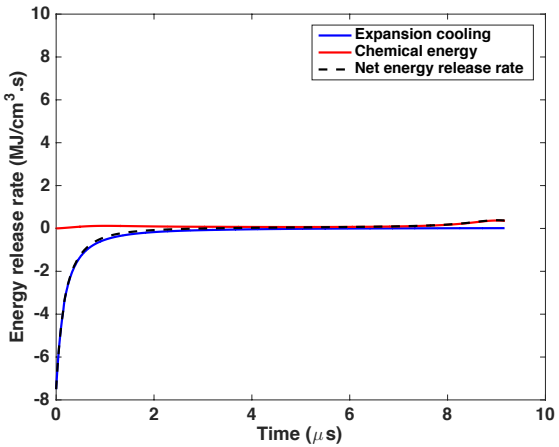
Chemical energy vs Cooling (expansion)

Sub-critical



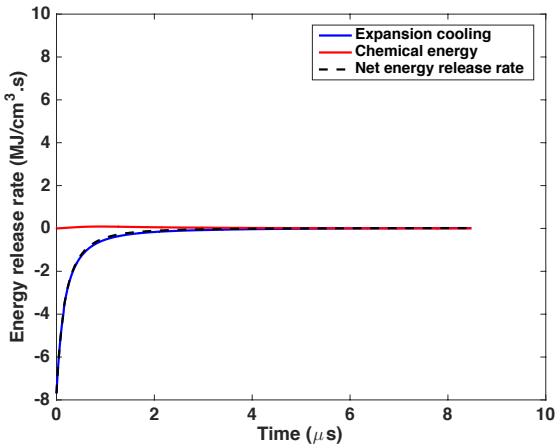
200 K/τ

Near-critical



225 K/τ

Super-critical



230 K/τ

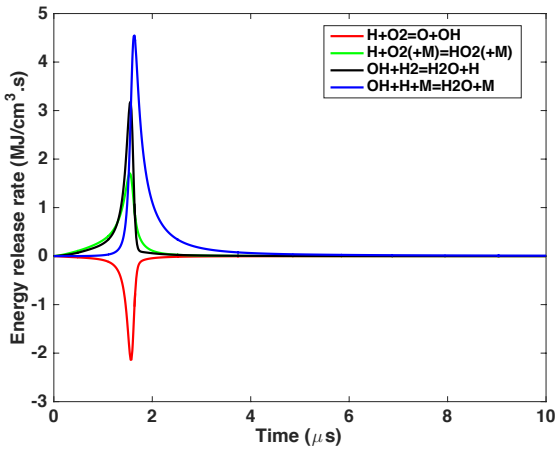
At 225 K/τ, weak energy release at longer time

At 230 K/τ, no significant energy release

Energy release per reaction

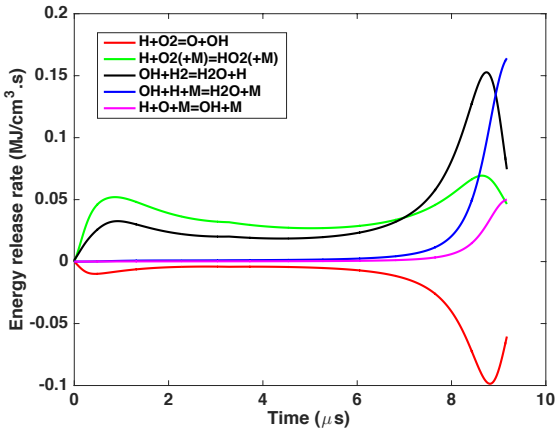
Focus on chemical energy release

Sub-critical



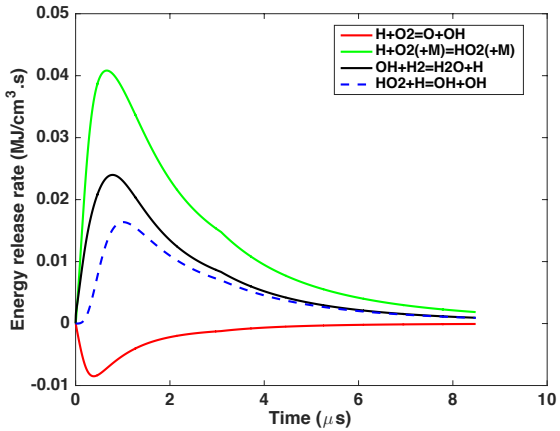
200 K/τ

Near-critical



225 K/τ

Super-critical



230 K/τ

At $\leq$ 225 K/τ :

Induction : $H+O_2(+M) = HO_2(+M)$

Exothermic : $OH+H_2 = H_2O+H$ and $OH+H(+M) = H_2O(+M)$

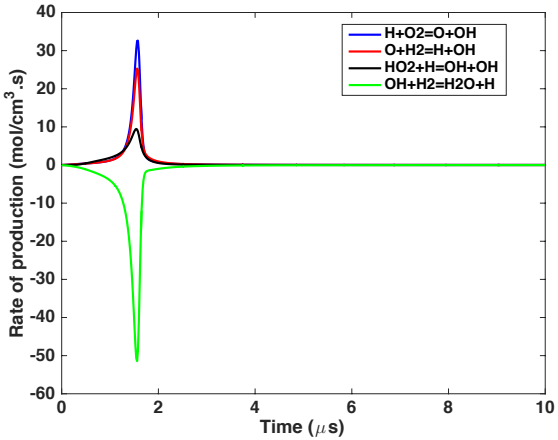
At $>$ 225 K/τ :

No switch to branching chemistry

Rate of production

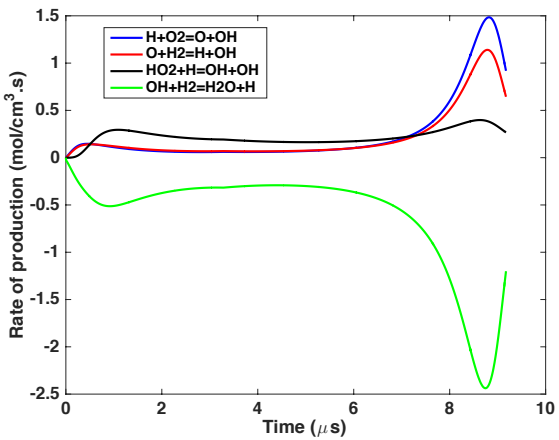
Analysis for OH radical

Sub-critical



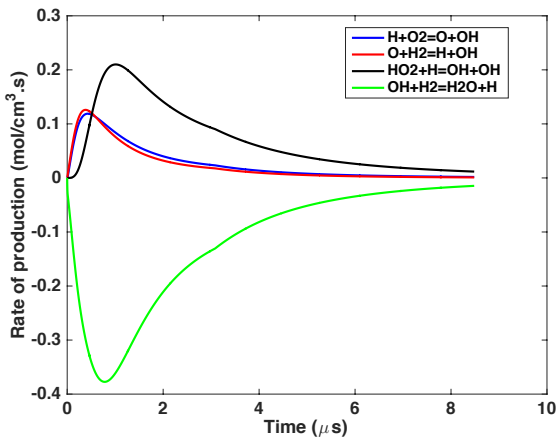
200 K/τ

Near-critical



225 K/τ

Super-critical



230 K/τ

At $\leq$ 225 K/τ :

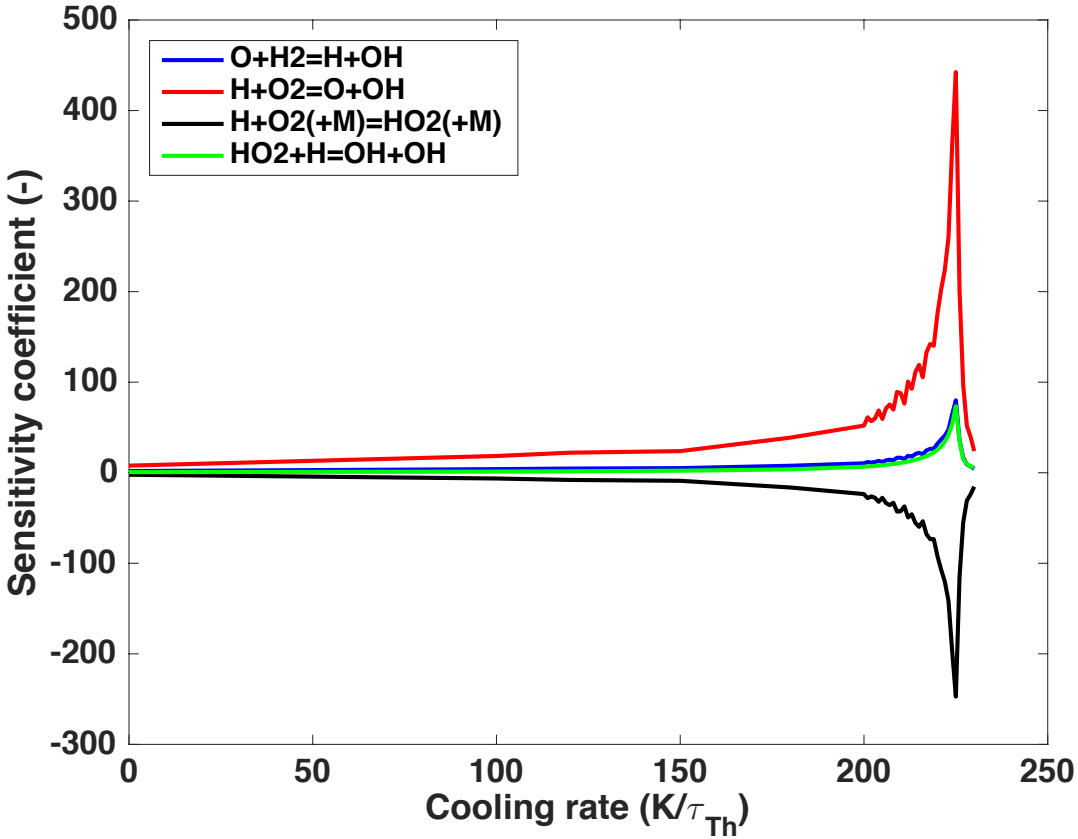
Double inversion between linear chain and chain branching

At $>$ 225 K/τ :

Single inversion between linear chain and chain branching

Sensitivity coefficient on OH

Evolution as a function of cooling rate



Increasing sensitivity and competition between linear chain and chain branching

outlines

Conclusion

Study of chemical kinetics of hydrogen-air mixtures under volumetric expansion

- **Power law decay is the least efficient at quenching the reaction**
- **Intermediate pressure (P_1 = 500-800 kPa) are the most sensitive to quenching**
- **Low pressure (P_1 < 100 kPa) are the least sensitive to quenching**
- **Complex response to expansion is due to the extended second explosion limit**

Acknowledgments

Thank you for your attention

Questions ?