FLAME CHEMISTRY, DYNAMICS AND MODEL REDUCTION

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Research summary

1. Fuels

- $H_2/CH_4/CO/O_2$ flame speed (25 atm)
- Methyl-butanoate (extinction & transport)
- t-butanol (extinction)

2. Model reduction

- Dynamic multi-timescale
- Multi-generation path flux analysis
- Adaptive chemistry

3. Theory and modeling

- Minimum ignition energy
- Multi flame regimes and critical ignition temperature gradient in HCCI combustion

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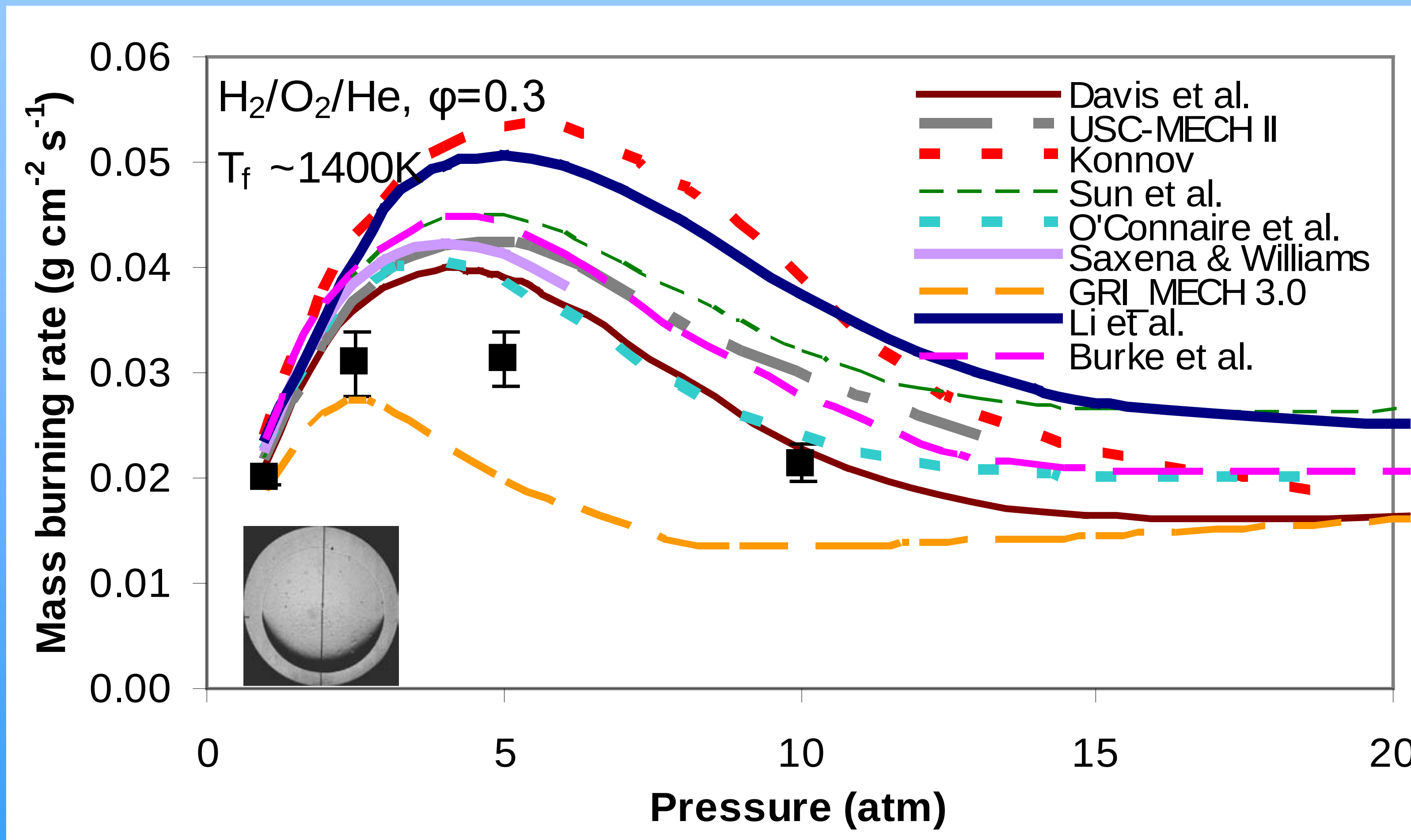
Fuel: Hydrogen mechanism and negative pressure dependence



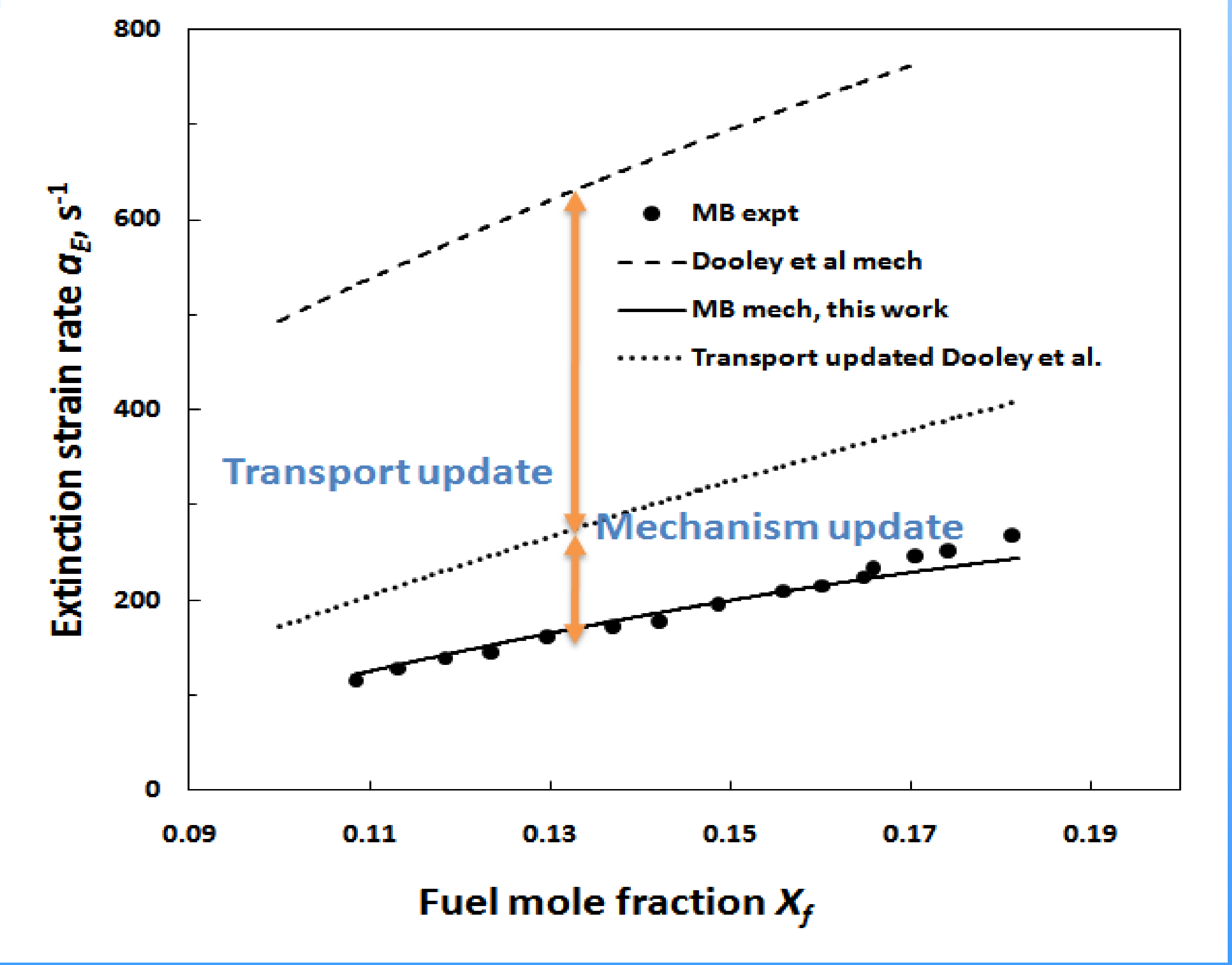
$HO_2+OH=H_2O+O_2$

$HO_2+H=OH+OH$

$H+O_2+M=HO_2+M$

Increasing sensitivity with pressure

Fuel: Methyl butanoate: kinetic validation and transport



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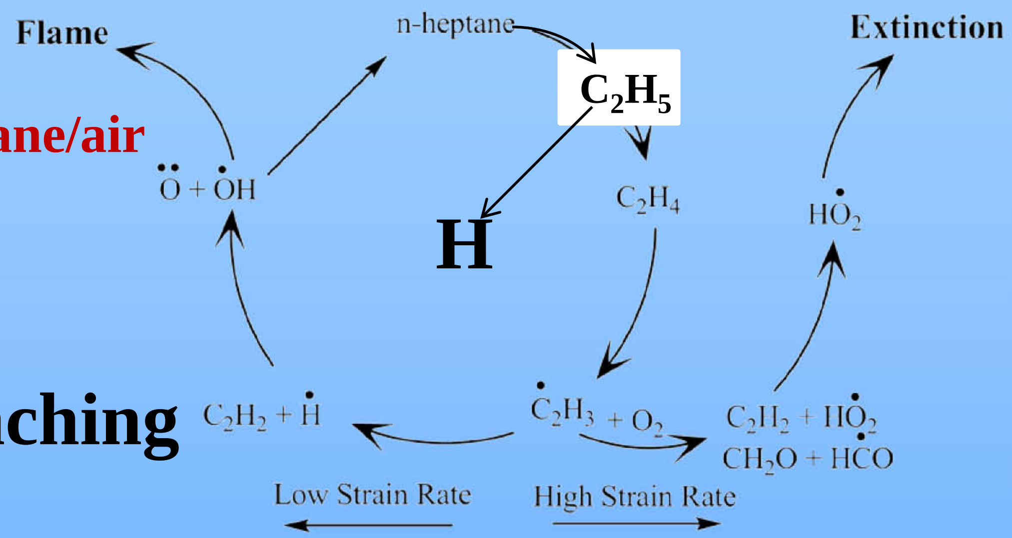
Impact of Functional Groups on Flame Chemistry

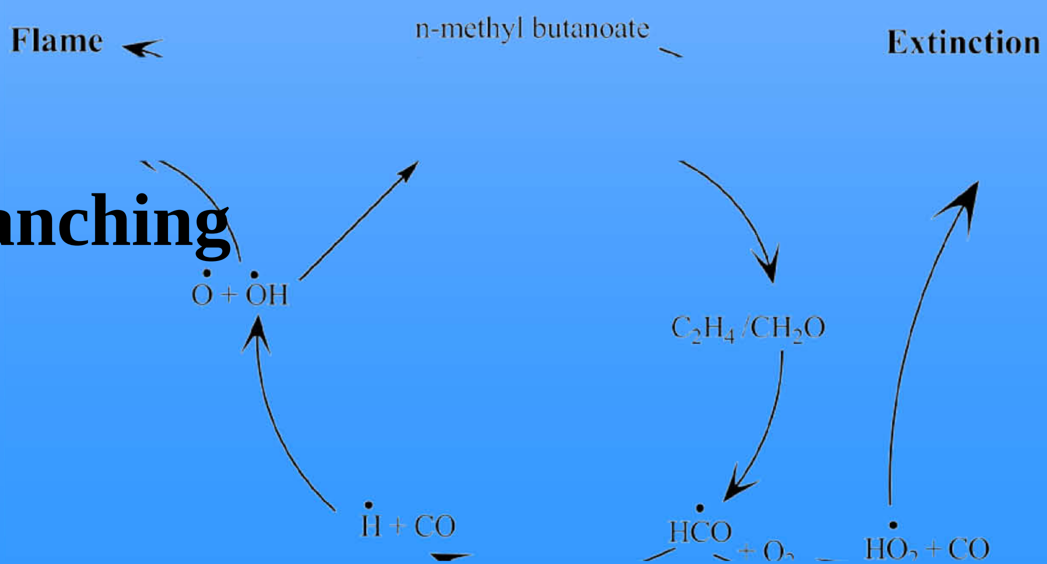
N-heptane/air

Branching **Termination**



Methyl-butanoate/air

Branching **Termination**



Uddi, Dooley, Won, Dryer, and Ju, CF, 2010

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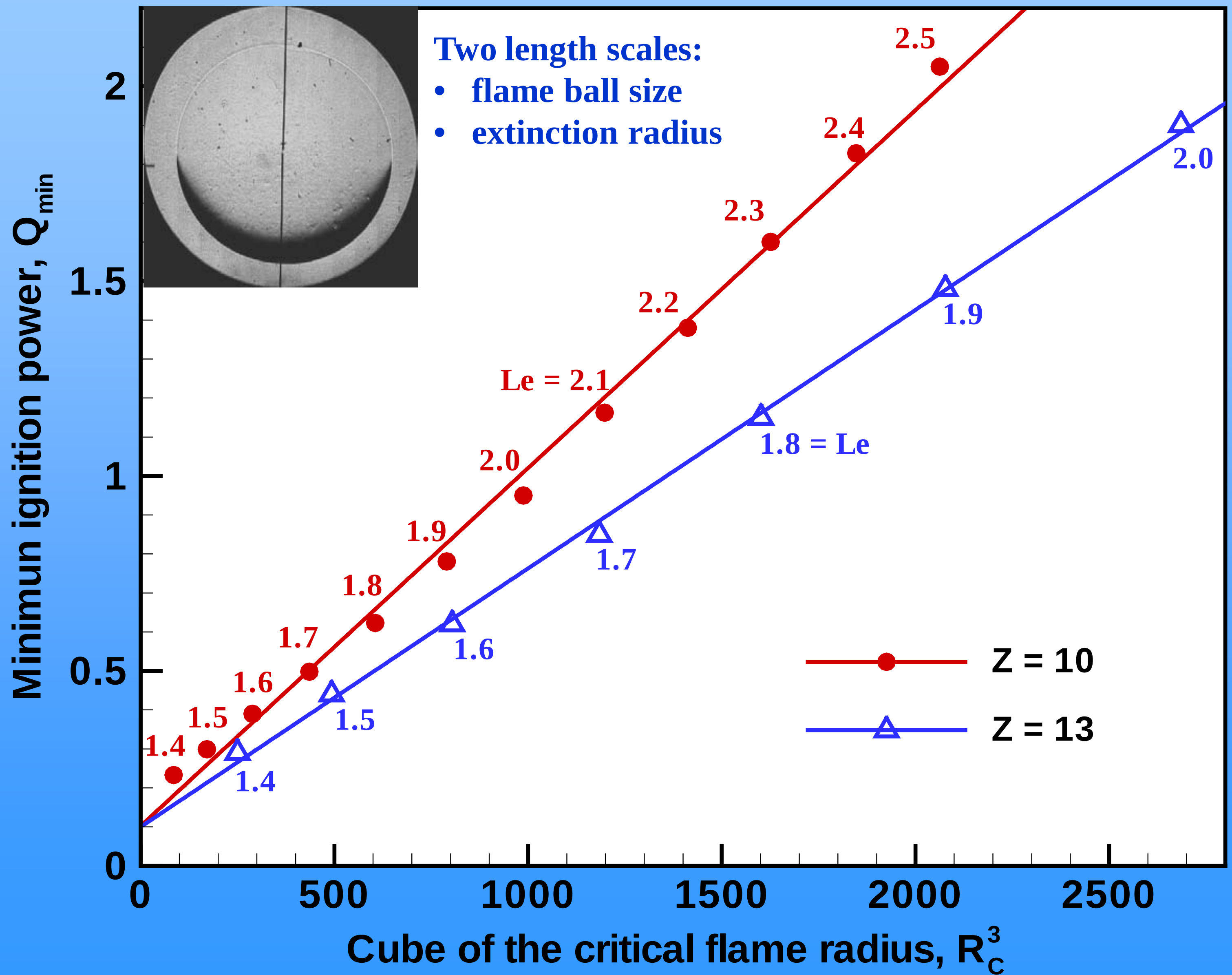
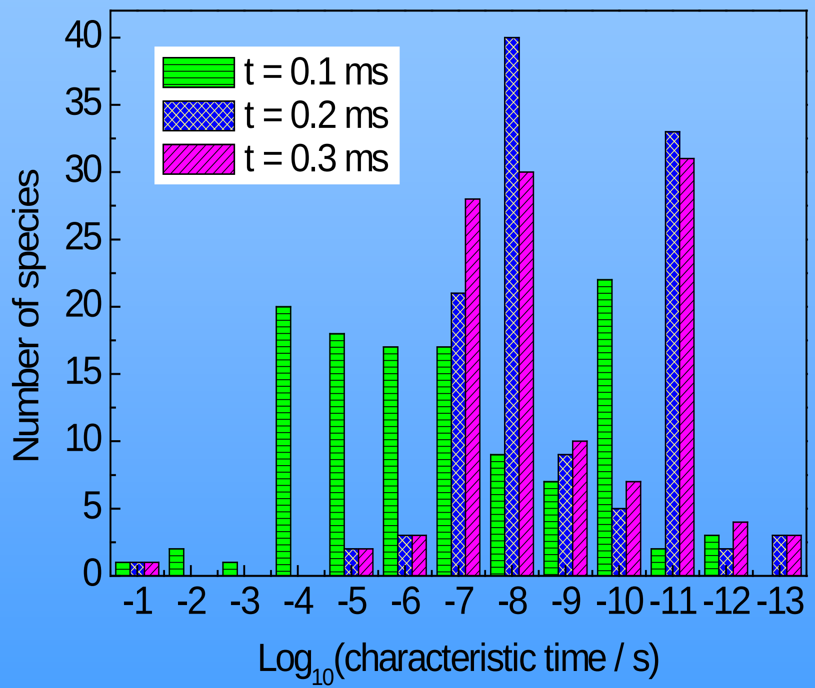
Theory: Minimum ignition energy vs. critical flame radius



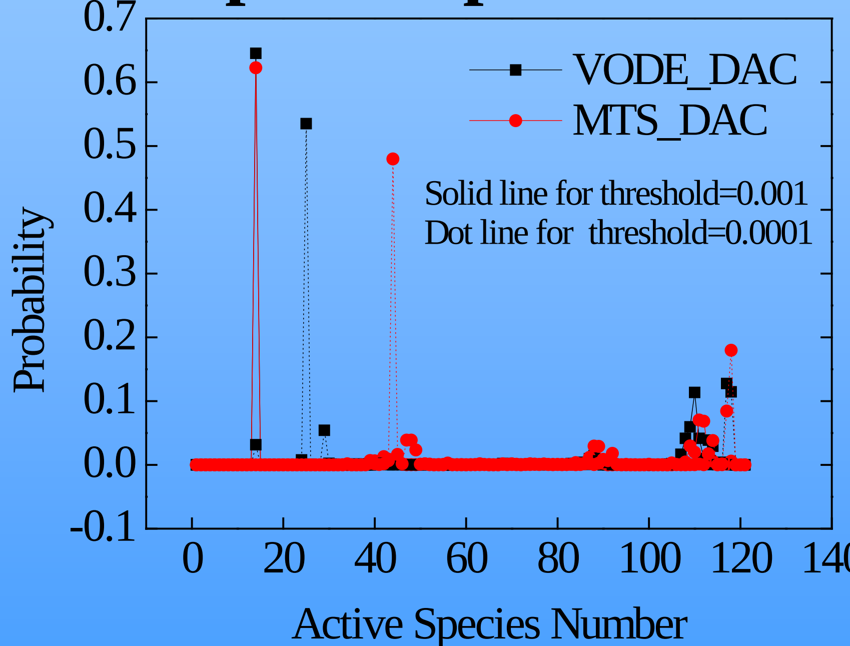
Model reduction:

Multi-scale nature in n-heptane ignition

Time space



Species space

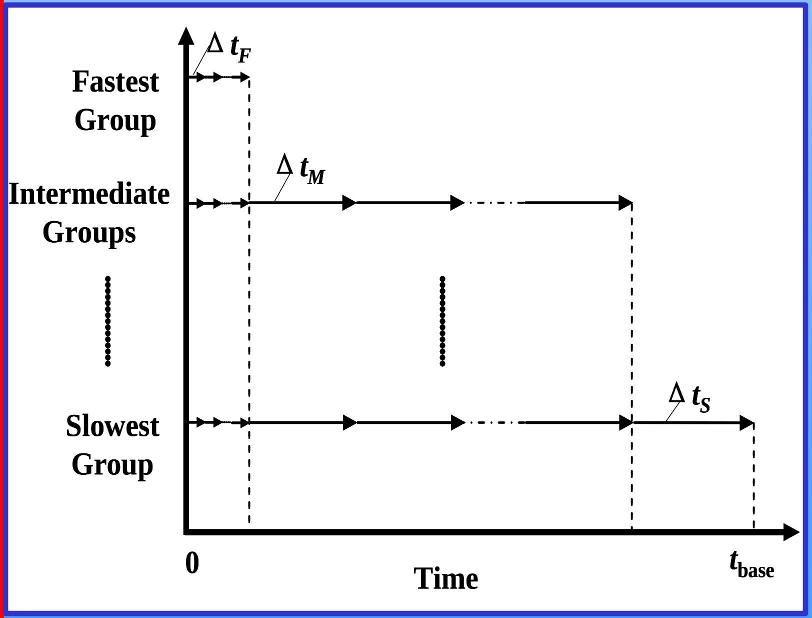


- Efficient and accurate multi timescale ODE integrator
- Efficient and dynamic reduction mechanism/tabulation

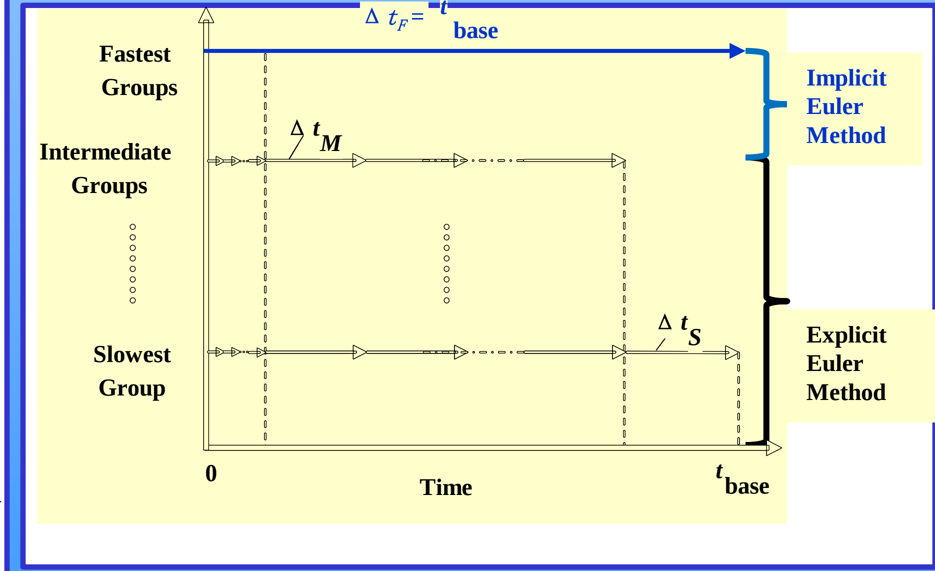
Gou et al. CF, 2010

A new multi-timescale method

- Dynamic multi-timescale



- Hybrid multi-timescale



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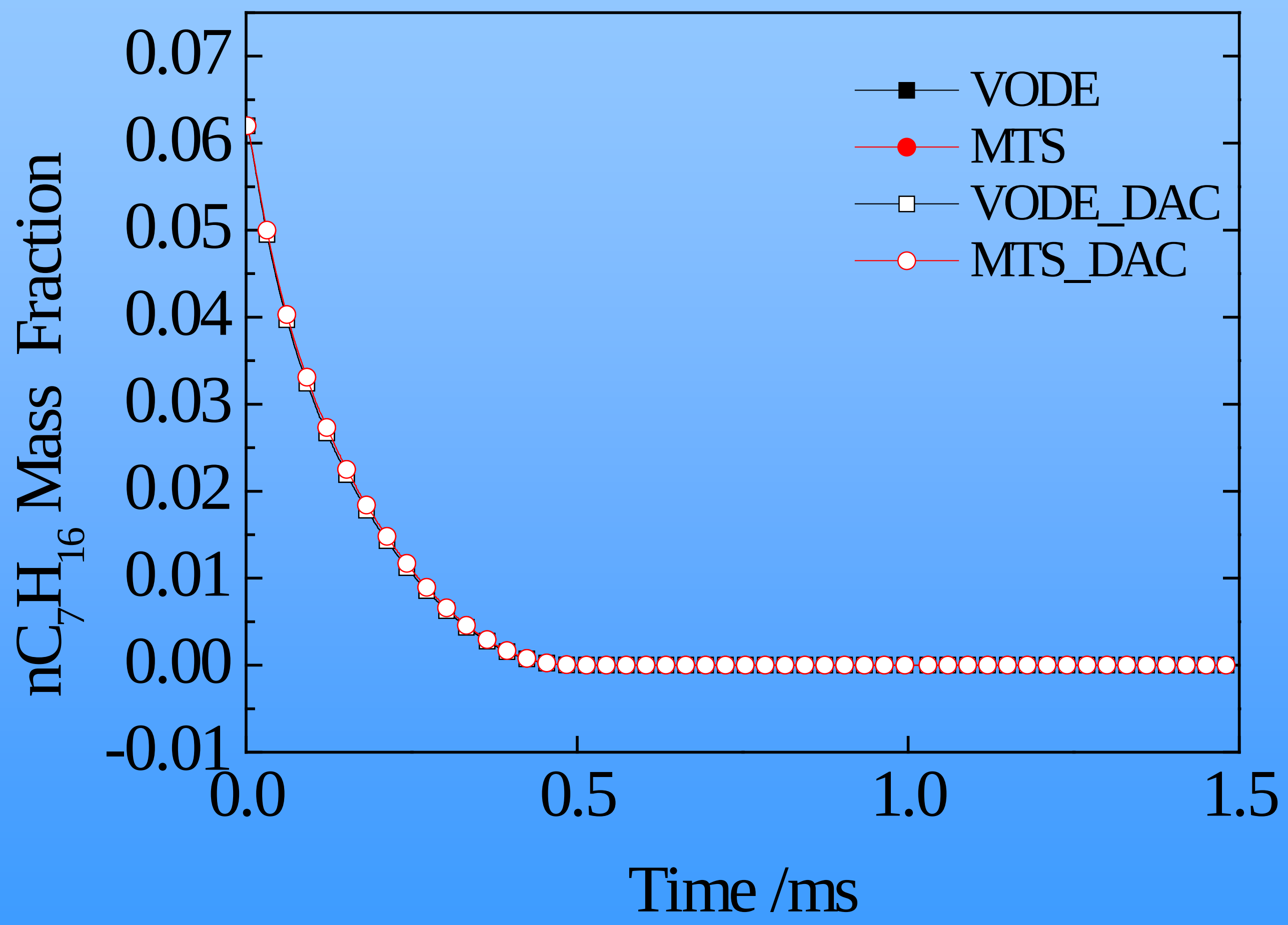
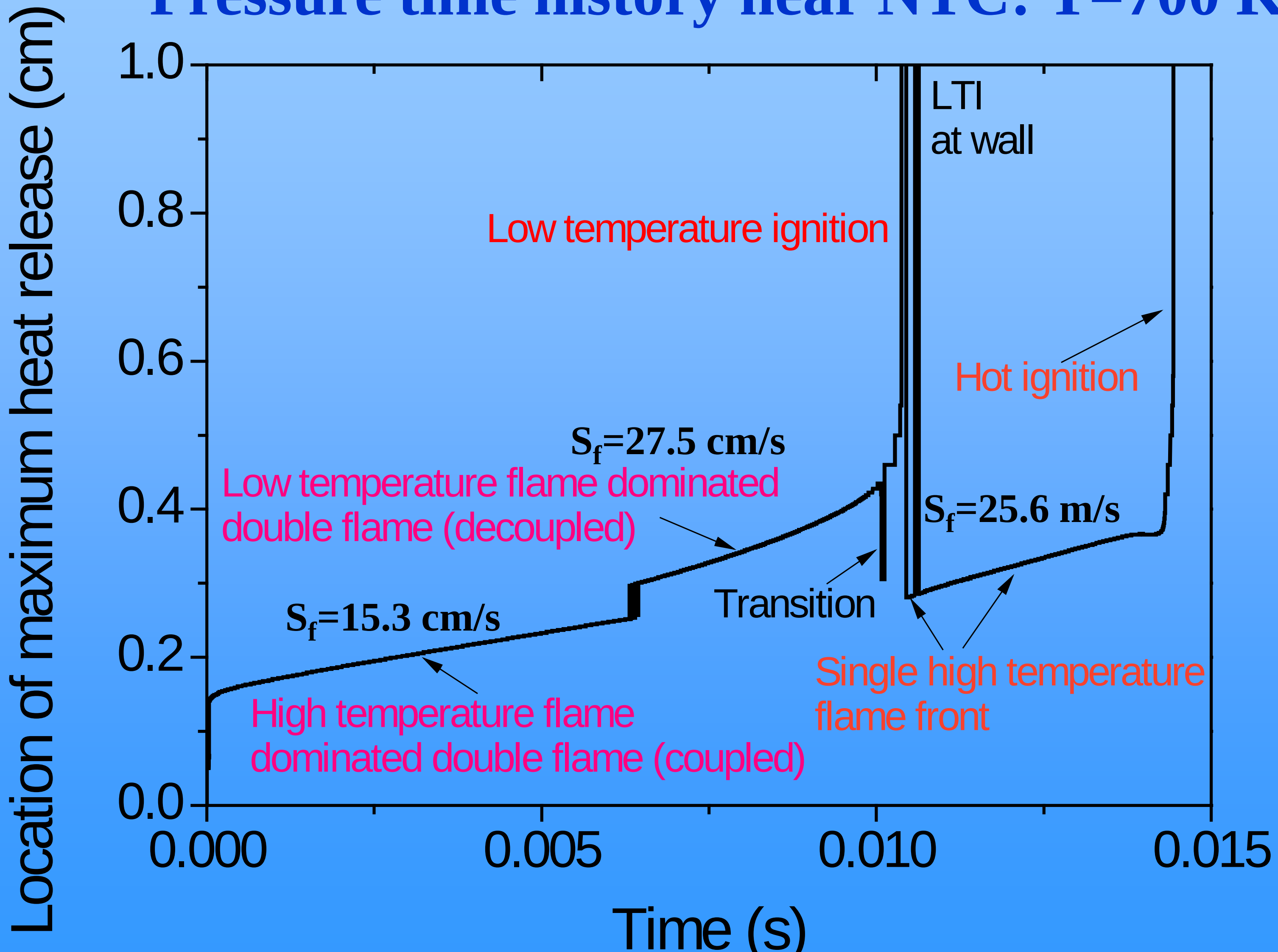
Integration of MTS with dynamic adaptive chemistry



Profiles of temperature and n-heptane mass fractions using n-heptane mechanism (160 species).

MTS modeling of HCCI: New flame regimes

Pressure time history near NTC: T=700 K



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Ignition front & acoustic wave coupling

Ignition wave speed:

$$u_{ig} = (\frac{\partial \tau}{\partial r})^{-1} = (\frac{\partial \tau}{\partial T}\frac{\partial T}{\partial r} + \frac{\partial \tau}{\partial \phi}\frac{\partial \phi}{\partial r})^{-1}$$

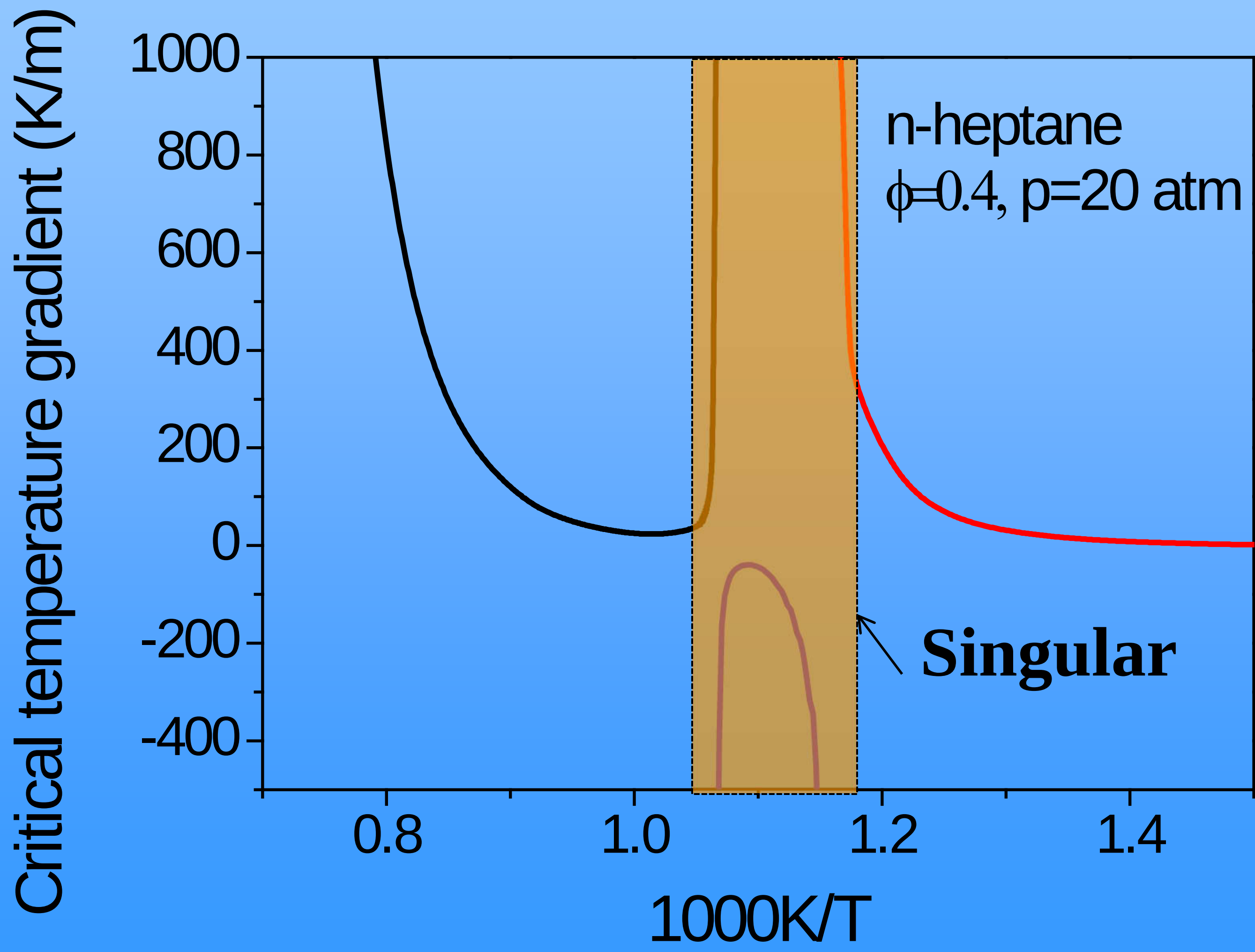
Ignition wave speed=acoustic speed

$$u_{ig} = a: \qquad \frac{\partial T}{\partial r}\Big|_c = (a\frac{\partial \tau}{\partial T})^{-1}$$

$$\xi = \frac{\partial T}{\partial r} / \frac{\partial T}{\partial r}\Big|_c \Rightarrow \begin{cases} >1 \text{ Subsonic ignition wave, deflagration} \\ \sim 1 \text{ developing detonation} \\ <1 \text{ Supersonic ignition wave} \end{cases}$$

Acoustic timescale: t/R

NTC effect on critical temperature gradient



Conclusion

- Negative pressure dependence and uncertainty of hydrogen mechanism at high pressure and low temperature
- Transport effect and kinetic coupling between n-heptane/methyl butanoate were identified.
- Multi-timescale modeling with adaptive chemistry was developed.
- New flame regimes due to NTC at HCCI conditions were identified.
- At the NTC region, the critical temperature gradient for ignition and flame front coupling becomes singular.