Direct Numerical Simulation of Ignition and Combustion under Extreme Conditions

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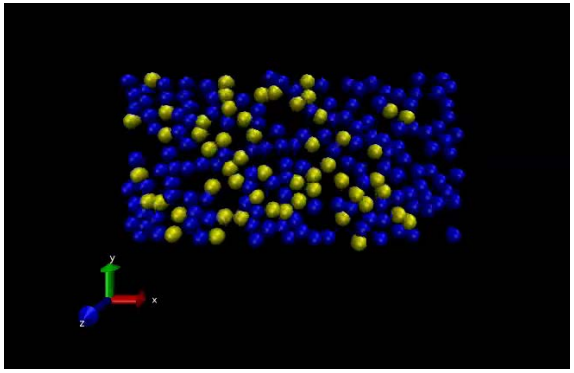

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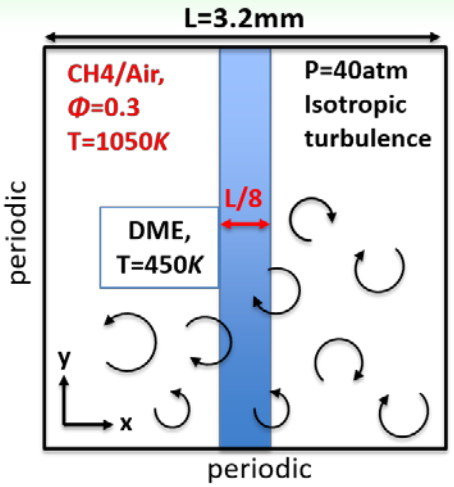
Ignition in Dual-fuel Mixture under High Pressure

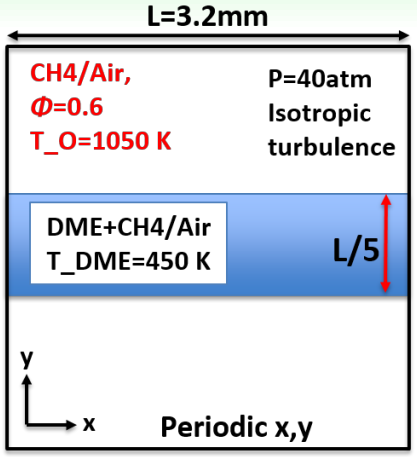
Configuration 1:
Pilot-ignited
DME/CH4-air



ξ∈(0,1)
Single ∇ ξ

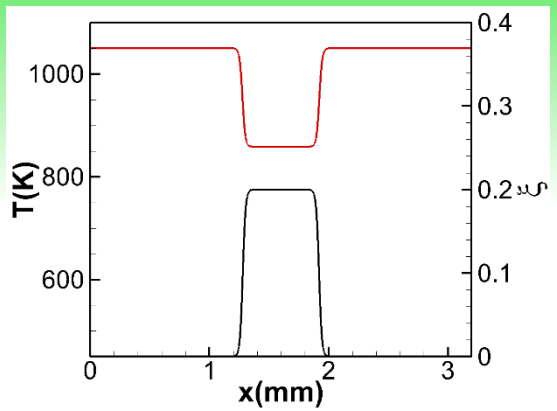
Tai Jin et al., PCI (2018)

Configuration 2:
Partially mixing
Relevant to RCCI



ξ∈(0,0.2), ξ∈(0,0.4)
Various ∇ ξ

Tai Jin et al., Applied Energy (2019)



Initial scalar profile across mixing layer

Mixture fraction: $\xi = (Y_{N2} - Y_{N2,o})(Y_{N2,f} - Y_{N2,o})$

Initial scalar profiles: $\delta = 24\ \mu m$

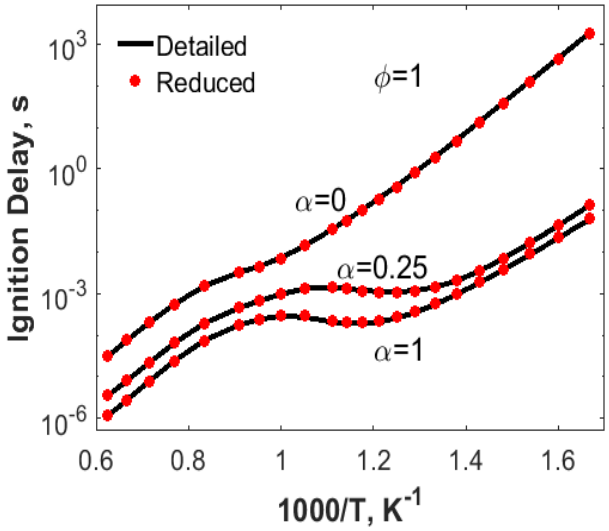
$$f(x) = \left(\frac{f_1+f_2}{2}\right)+\left(\frac{f_1-f_2}{2}\right)\tanh\left(abs\left(\frac{x-x_c}{\delta}\right)\right)$$

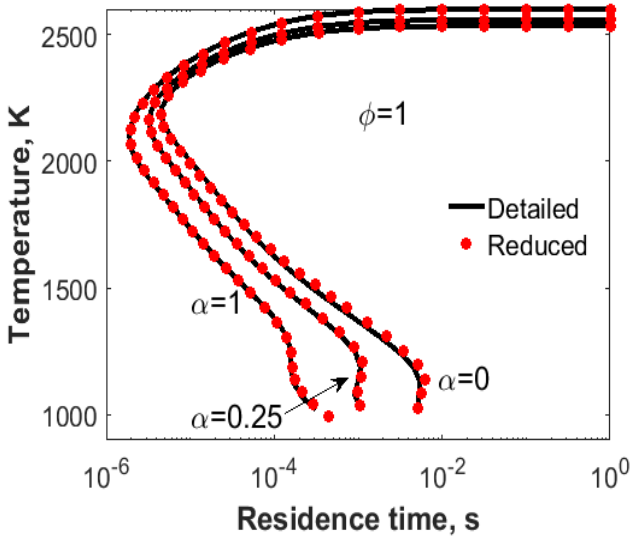
Initial turbulence fluctuations:

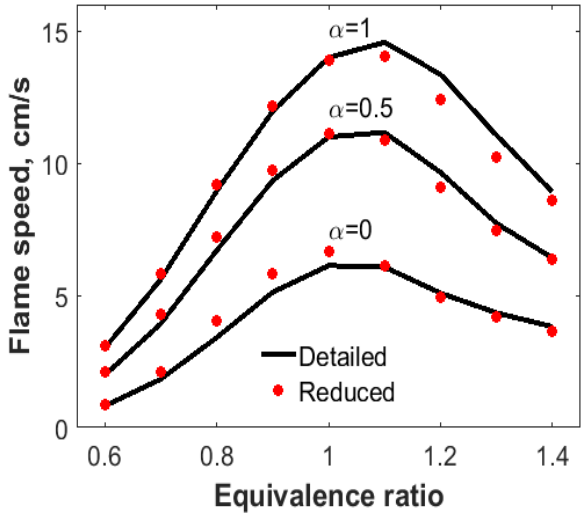
$$E(k) = \frac{32}{3}\sqrt{\frac{2}{\pi}}\frac{u'^2}{k_e}\left(\frac{k}{k_e}\right)^4 exp\left[-2\left(\frac{k}{k_e}\right)^2\right]$$

Chemical Mechanisms

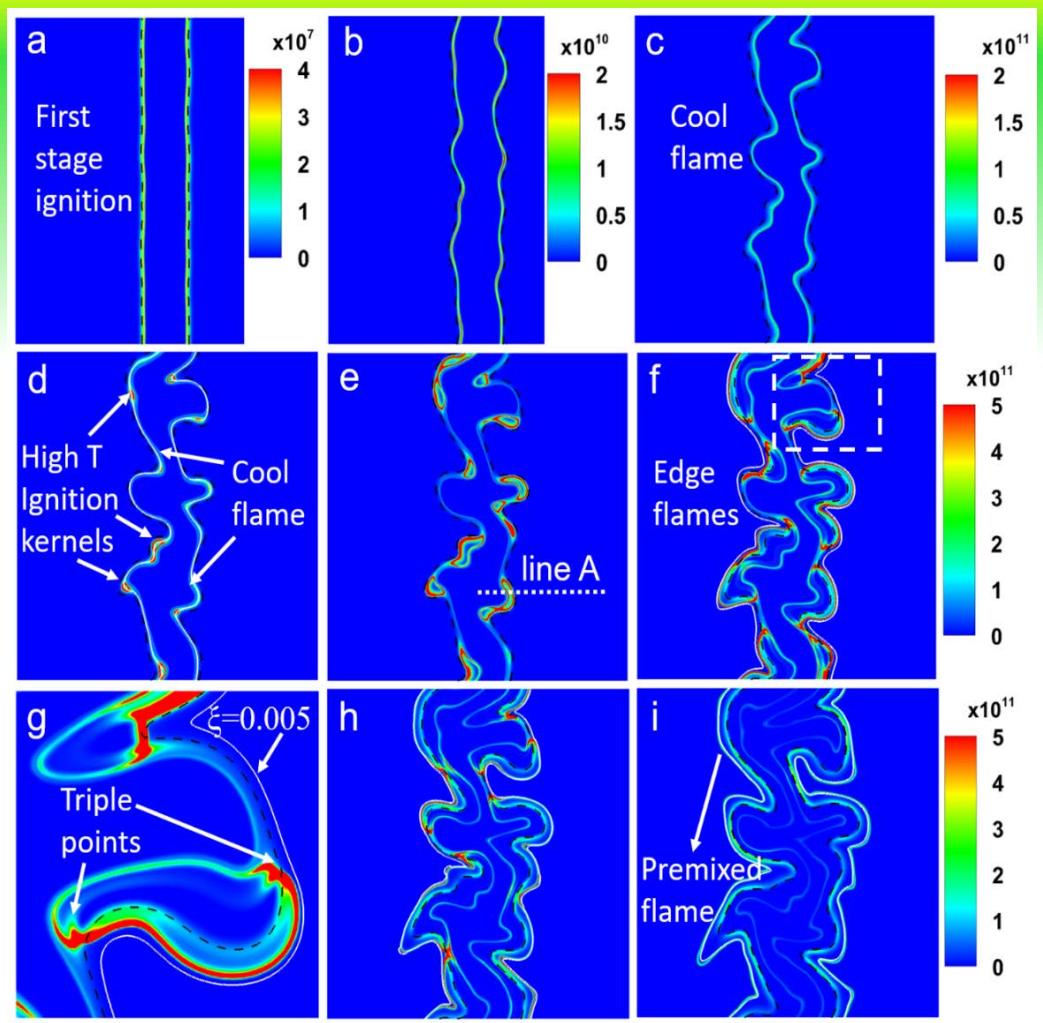
- Reduced by Tianfeng Lu from a validated detailed DME/CH_4 mechanism (Mech_56.54) by Henry Curran (2015)
- 25 species in 147 reaction steps
- Validated in ignition delay time, perfectly stirred reactor (PSR) extinction residence time, laminar premixed flame speed







Sample Results (Ignition Case 1)



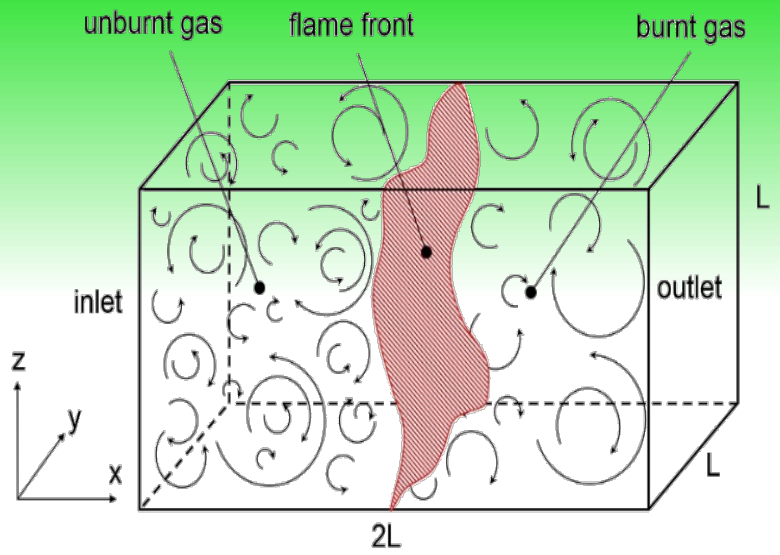
HRR (W/m^3), at 0.008, 0.06, 0.16, 0.23, 0.25, 0.29, 0.29, 0.33 and 0.41 ms

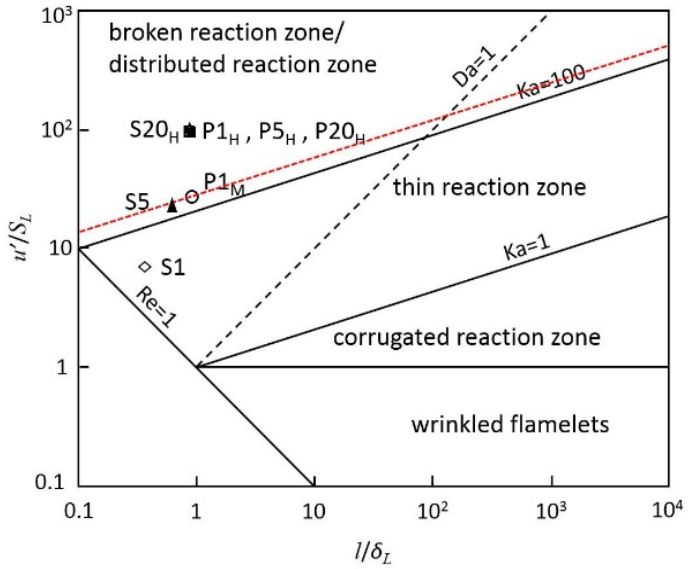
Case 1, φ=0.3, ξ_{max}=1.0, L_t=0.2 mm

- First stage ignition (LT) transits to propagating cool flame
- High T ignition kernel discretely located in fuel rich mixture
- Triple flames propagating along the ξ_{st} line
- Lean premixed branch initiates the premixed methane-air flame

Jin et al. Dynamics of triple-flames in ignition of turbulent dual fuel mixture: a direct numerical simulation study, PCI, 2018.

DNS of Turbulent Hydrogen Flames





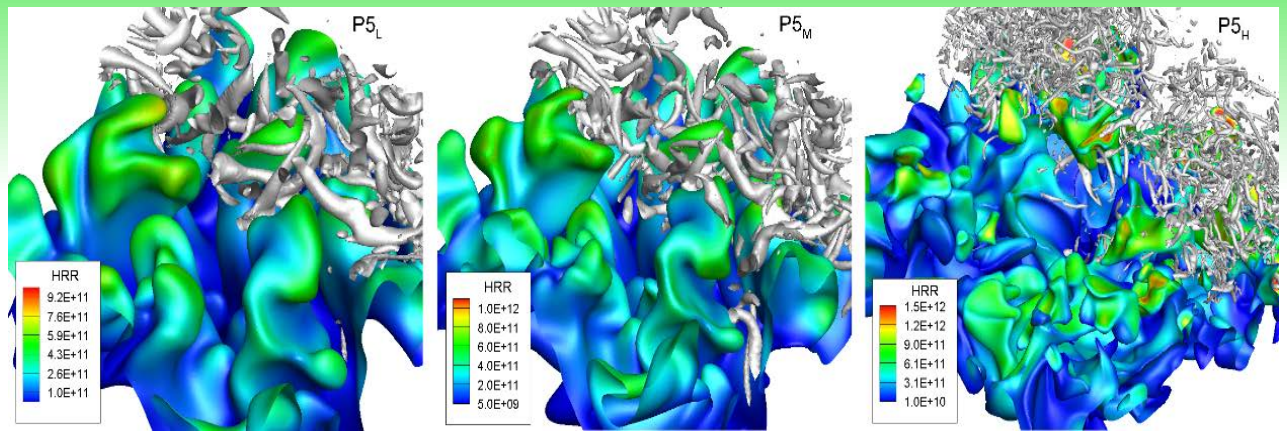
Simulation Conditions

- Karlovitz number up to 2335
- Pressure up to 20 atm
- Equivalence ratio down to lean limit
- A wide range of turbulent integral length scales

X. Wang, T. Jin and K. H. Luo, International Journal of Hydrogen Energy 44 (5): 3195-3207 (2019).

DNS of Turbulent Hydrogen Flames

Ka Effects

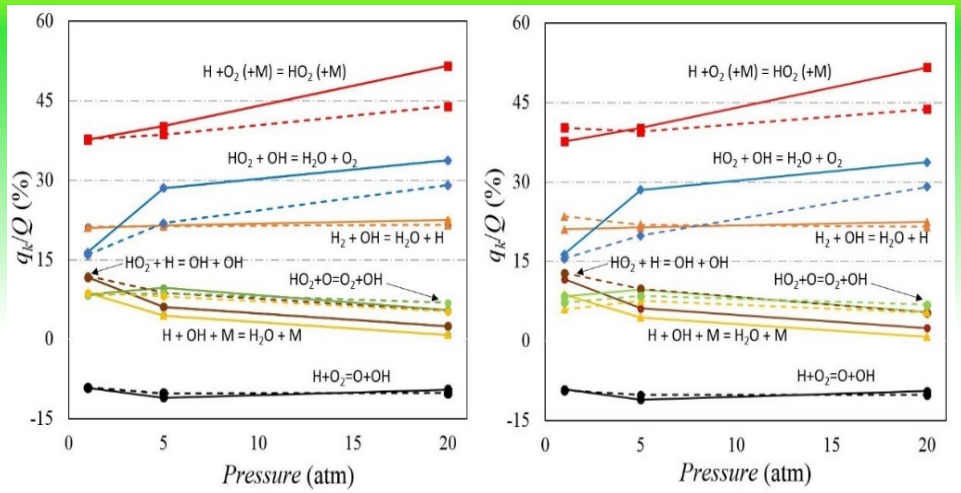


- At high Ka, the flame fronts are seriously wrinkled with vortices existing within the reaction zone.
- At elevated pressure, small eddies could not survive across the reaction zone.

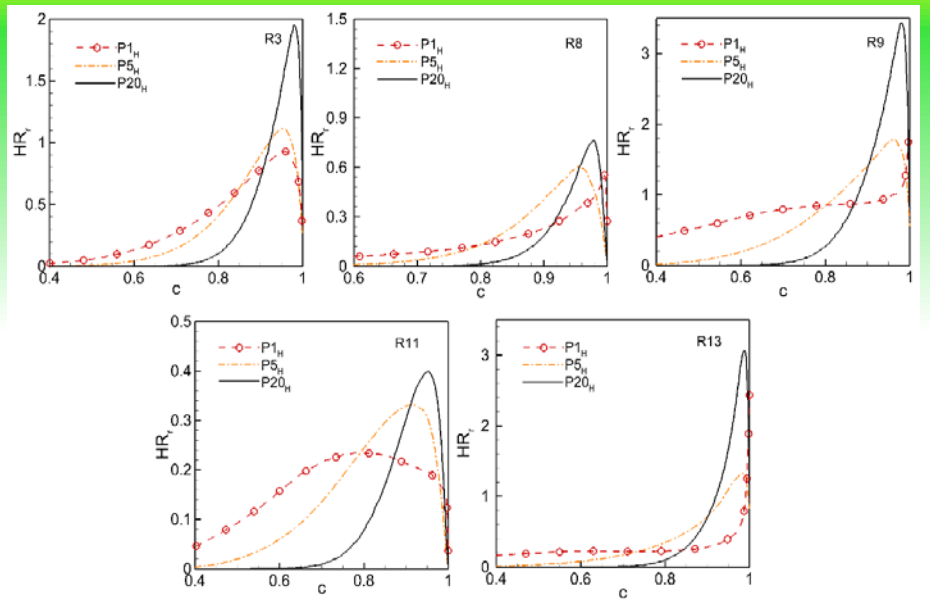
X. Wang, T. Jin and K. H. Luo, International Journal of Hydrogen Energy 44 (5): 3195-3207 (2019).

DNS of Turbulent Hydrogen Flames

Pressure Effects



Heat release contributions of elementary reactions against pressures for both laminar (solid lines) and turbulent (dashed lines) flames.



Relative heat release contributions of individual elementary reactions versus progress variable for flames with the same Ka but different pressures.

- Laminar flames are more susceptible to elevated pressure than turbulent flames.
- The effects of pressure on global chemical pathways are more significant than those of Ka.
- With increasing pressure, active reaction zones seem to move to regions with high values of progress variable.

DNS of Realistic Reactive Systems

II. DBM Discrete Boltzmann Method

$$\frac{\partial f_i^{\sigma}}{\partial t}+v_{i\alpha}^{\sigma}\frac{\partial f_i^{\sigma}}{\partial r_{\alpha}}=\Omega_i^{\sigma}+G_i^{\sigma}+R_i^{\sigma}$$

Force term

Collision term

Reaction term

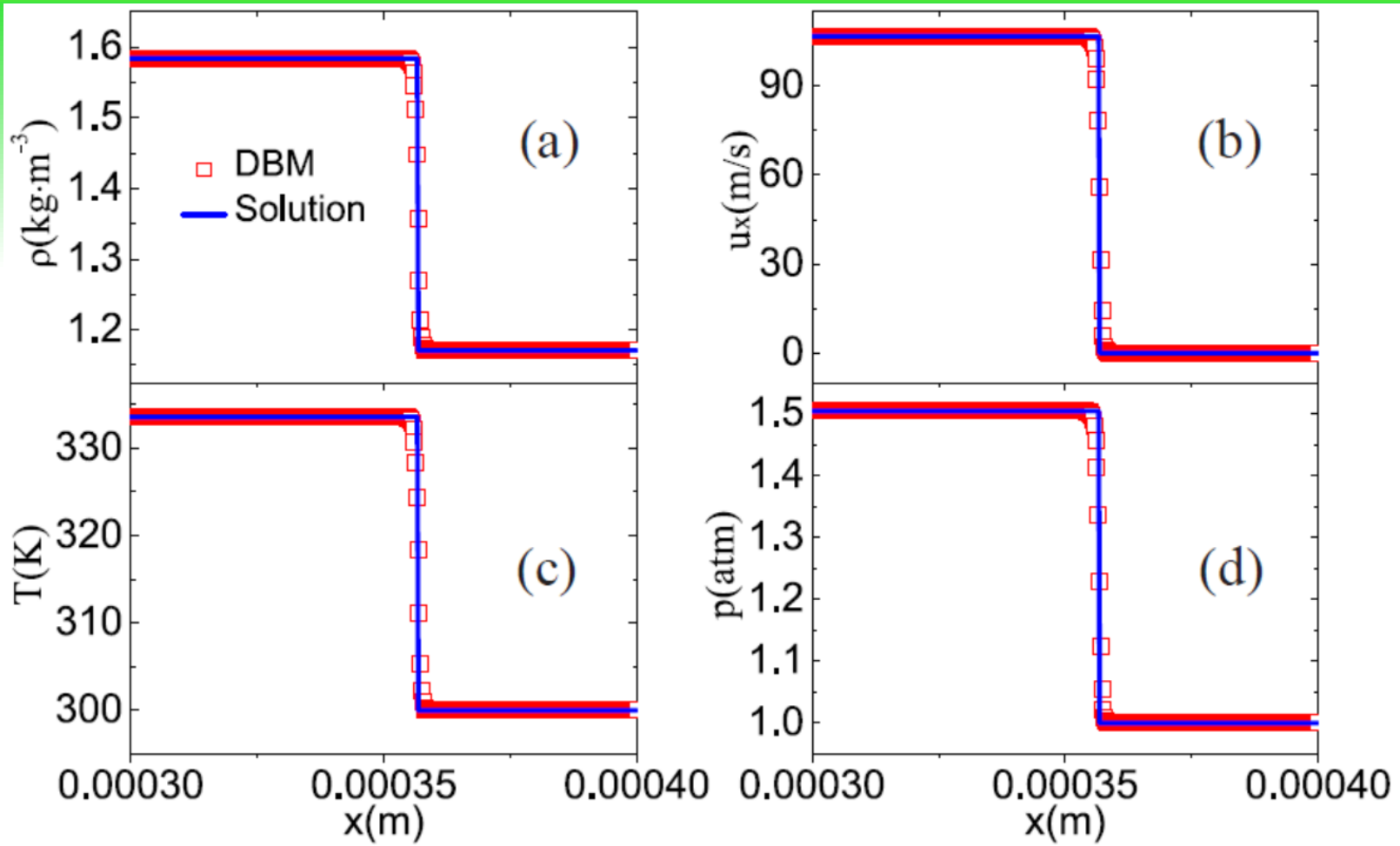
Force term $G_i^{\sigma}=\frac{1}{\tau^{\sigma}}\left[f_i^{\sigma eq}\left(n^{\sigma},\mathbf{u}^{\dagger\sigma},T^{\dagger\sigma}\right)-f_i^{\sigma eq}\left(n^{\sigma},\mathbf{u}^{\sigma},T^{\sigma}\right)\right]$

where velocity changes from $\mathbf{u}^{\sigma}$ to $\mathbf{u}^{\dagger\sigma}$ within time τ^{σ} due to external force, and temperature changes from T^{σ} to $T^{\dagger\sigma}$.

Reaction term $R_i^{\sigma}=\frac{1}{\tau^{\sigma}}\left[f_i^{\sigma eq}\left(n^{\sigma*},\mathbf{u},T^{*}\right)-f_i^{\sigma eq}\left(n^{\sigma},\mathbf{u},T\right)\right]$

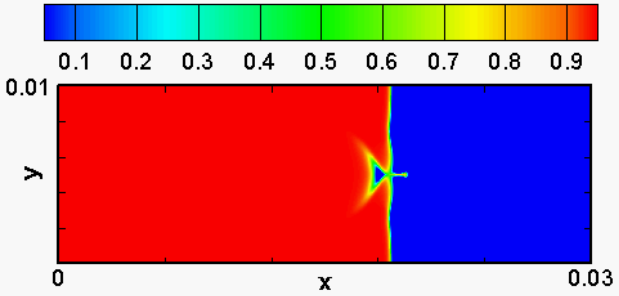
where number density changes from n^{σ} to $n^{\sigma*}$ within time τ^{σ} due to chemical reaction, and temperature changes from T to T^{*}.

II. DBM Discrete Boltzmann Simulation of Shock Wave

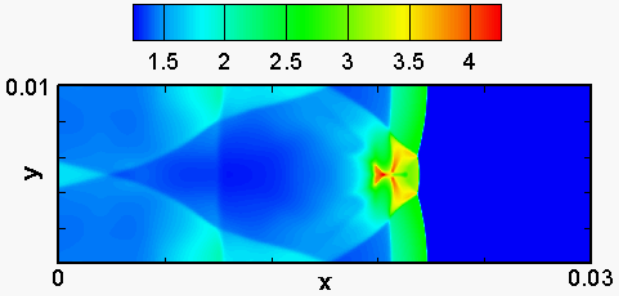


Discrete Boltzmann Simulation of Nonequilibrium Detonation

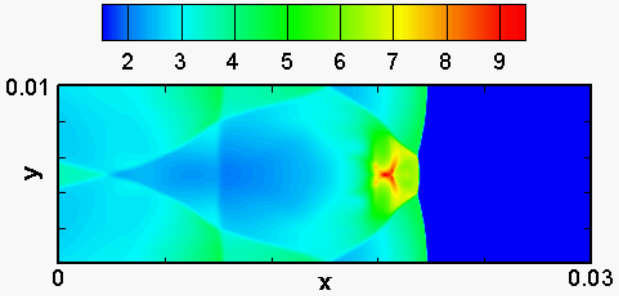
Reaction process



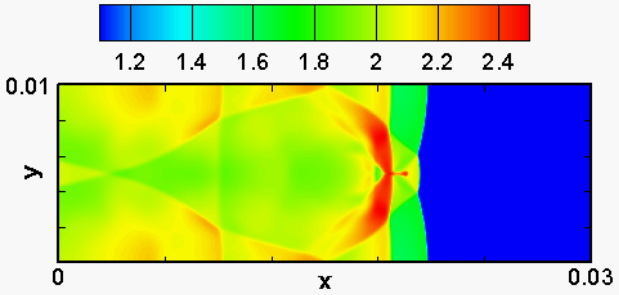
Density



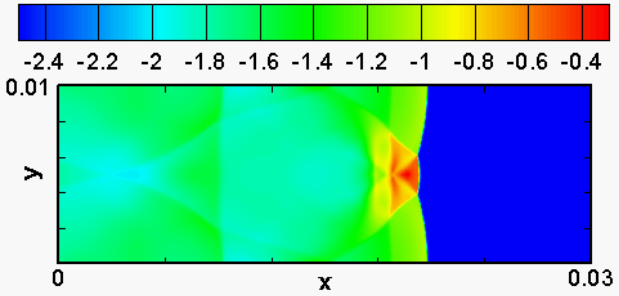
Pressure



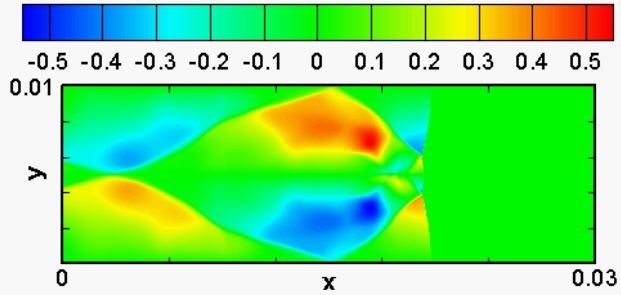
Temperature



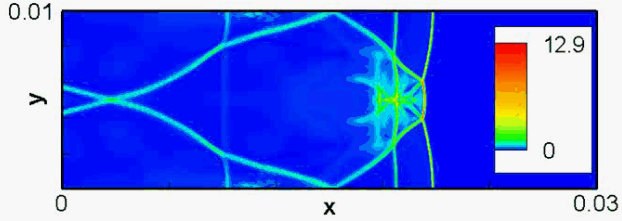
Horizontal velocity



Vertical velocity



Nonequilibrium



Summary

- **Ignition and combustion under extreme conditions has been studied using DNS.**
- **DNS of complex fluid-solid interaction and explosion is feasible.**
- **Lattice Boltzmann method is a viable alternative to DNS, with the possibility of providing “more physics”.**