2nd International Workshop on Near-Limit Flames
Beijing, China, July 27-28, 2019

Detonation initiation and propagation in non-uniform gaseous mixture

Peng Dai[1], Zheng Chen[2]

[1] Southern University of Science and Technology, China

[2] College of Engineering, Peking University, China

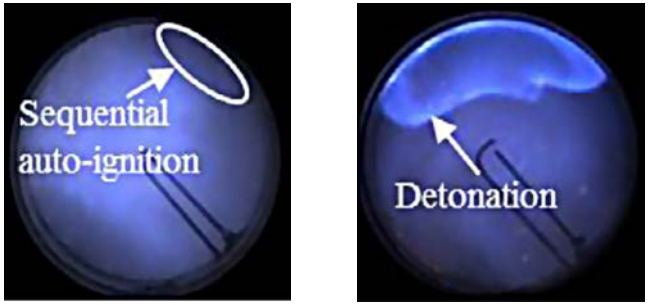
南方科技大学 SOUTHERN UNIVERSITY OF SCIENCE AND TECHNOLOGY

北京大学 Peking University

Background

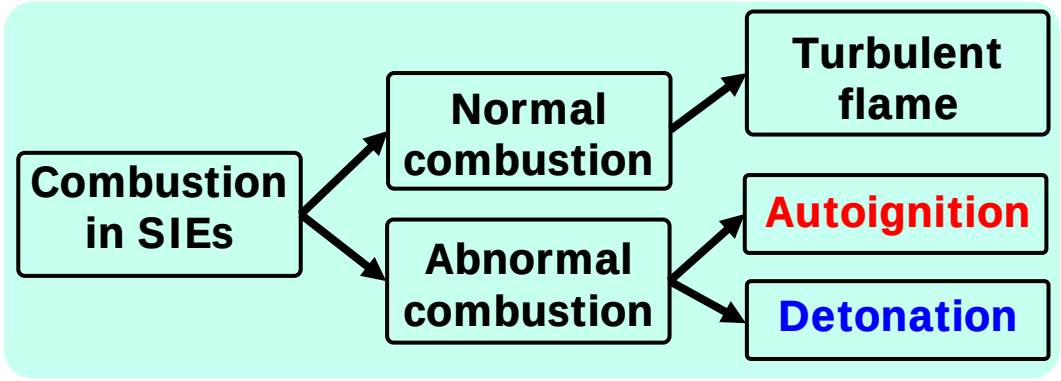
Autoignition in boosted SIEs

- Reactivity non-uniformity at high T & P
- End-gas autoignition/detonation
- Knock & Super knock

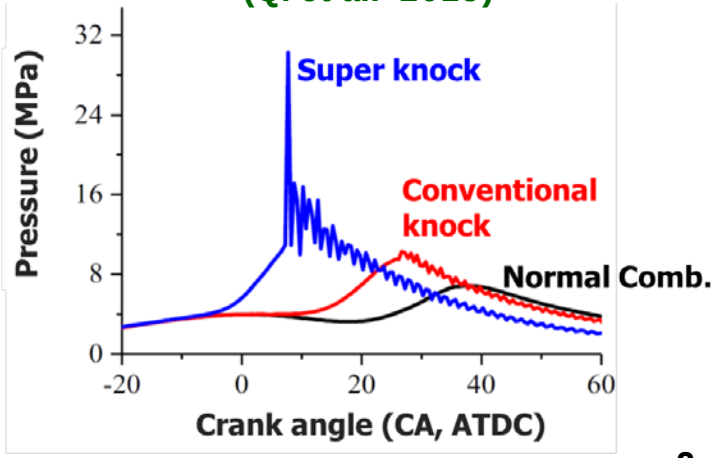


Conventional knock Super knock

(Qi et al. 2015)



(Wang et al. 2015, 2017)

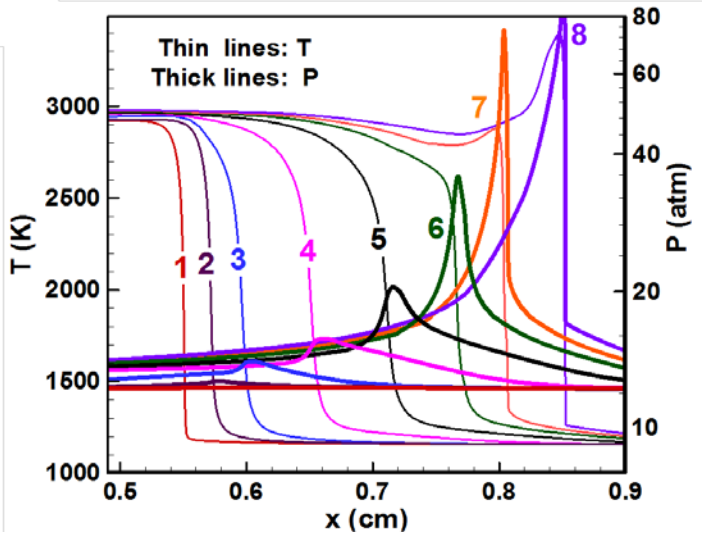


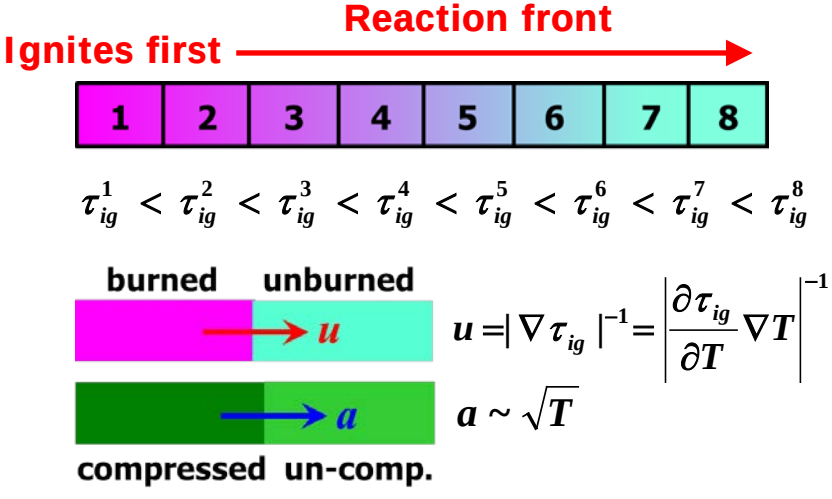
(Wang et al. 2015)

Autoignition with reactivity non-uniformity

Reactivity gradient (Zel'dovich), SWACER (Lee)

- Ignition delay: $\tau_{ig} = \tau_{ig}\left(T, P, \phi, Y_R\right)$
- Reaction front speed, *u* vs. Sound speed, *a*
- Detonation development: *u*~*a*

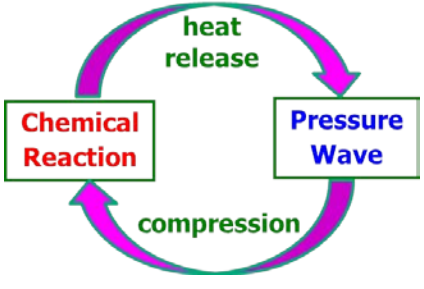




$$\tau_{ig}^1 < \tau_{ig}^2 < \tau_{ig}^3 < \tau_{ig}^4 < \tau_{ig}^5 < \tau_{ig}^6 < \tau_{ig}^7 < \tau_{ig}^8$$

$$u = |\nabla \tau_{ig}|^{-1} = \left|\frac{\partial \tau_{ig}}{\partial T}\nabla T\right|^{-1}$$

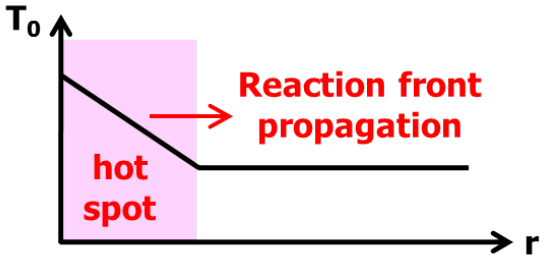
$$a \sim \sqrt{T}$$



Different modes of reaction front propagation

Analysis / simulation on hot spot

Zel'dovich 1980; Kapilar & Dold 1989; He & Clavin 1992, 1994; Weber 1994; Short 1997; Khokhlov et al. 1997; Kapila et al. 2002; Libermann et al. 2002; Radulescu et al. 2013; Ju 2017; Im 2019…

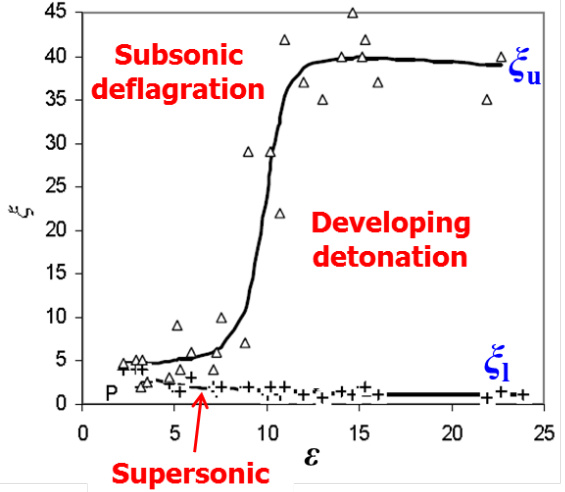


- Hot spot / compositional stratification
- Different autoignition modes

Detonation & engine knock

Bradley et al. 2002; Kalghatgi et al. 2012; Bates & Bradley 2016, 2017

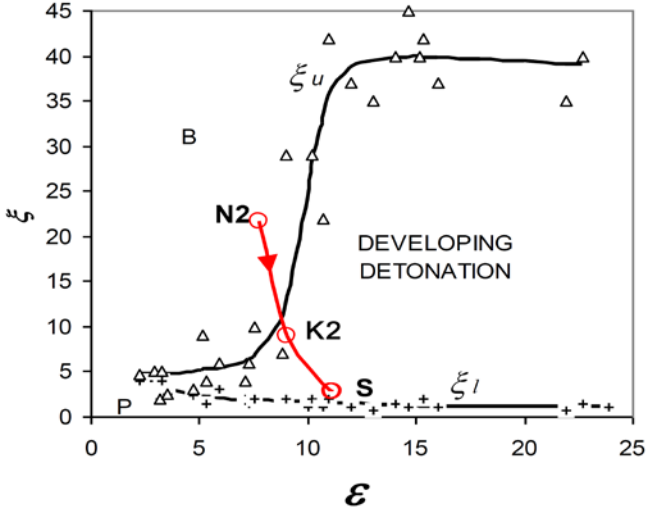
- Regime map in terms of ξ and ε
  - ✓ ξ : non-dimensional T gradient
  - ✓ ε : $(r_0 / a) / \tau_e$ time-scale ratio
- Detonation peninsular & engine knock

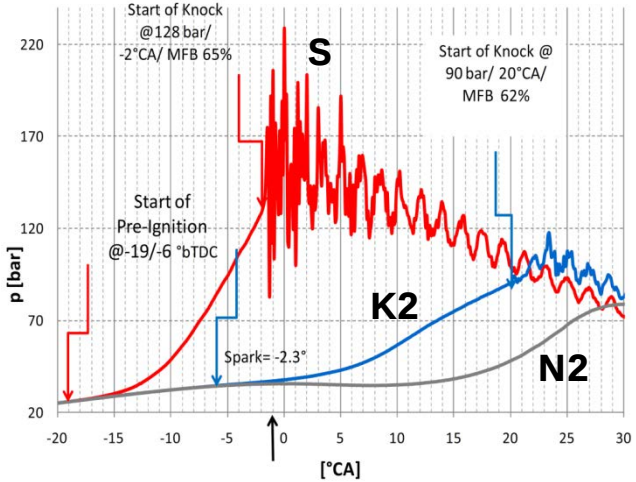


(Bradley et al. 2002)

Detonation and engine knock

Kalghatgi & Bradley 2012, 2015; Bates & Bradley 2016, 2017



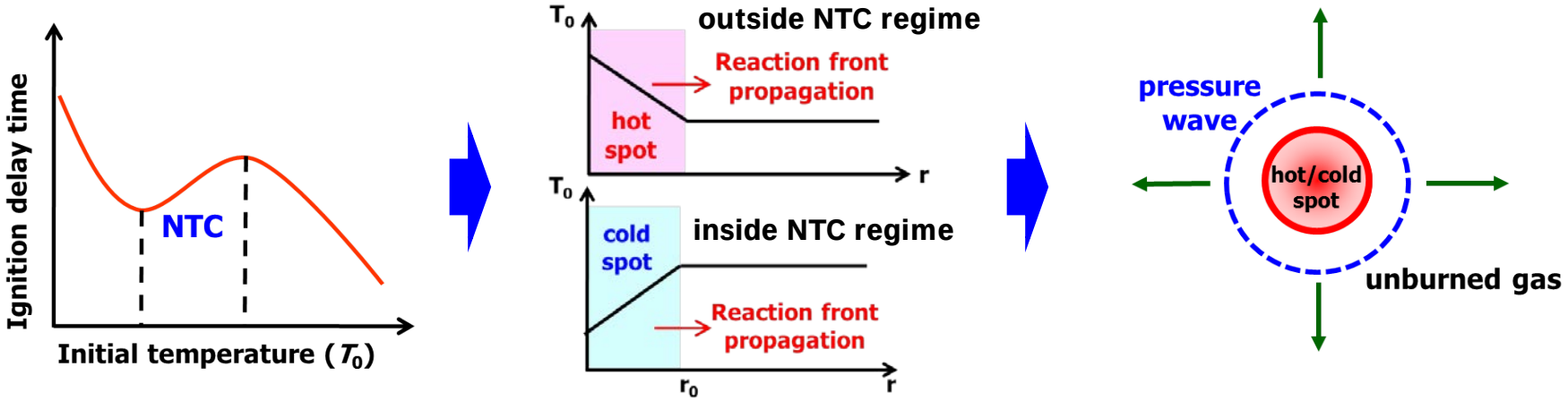


However, this detonation regime map was based on H_2/CO.

- **Can it be used for other fuels ?**
- **Is it affected by the initial temperature, pressure, equivalence ratio?**
- **What is the role of chemistry (low T chem. for large fuels) ?**
- **How about CO_2 dilution, with NOx … ?**

Objectives

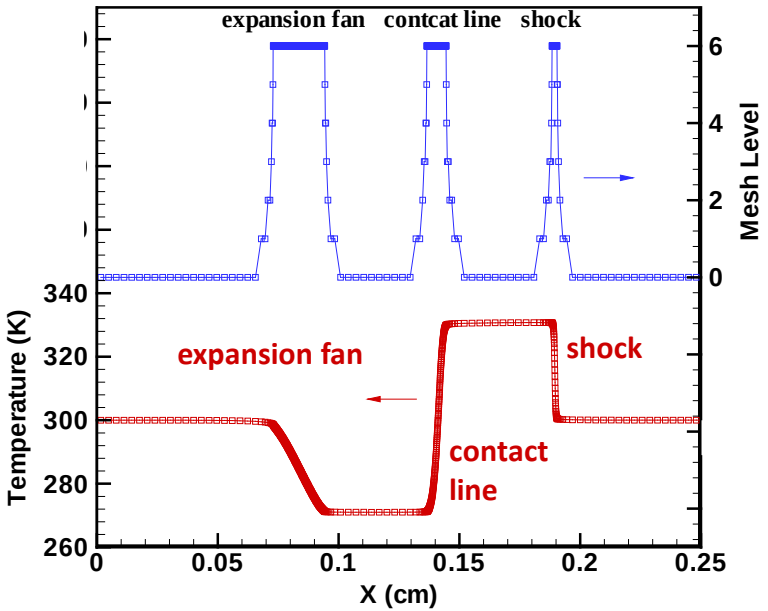
- To obtain detonation development regimes for fuels other than syngas
- To examine the effects of initial temperature, pressure and equivalence ratio on detonation development
- To assess the influence of low-temperature chemistry, CO_2 dilution, and NOx addition on detonation development



Numerical method

Solver: A-SURF (Adaptive Simulation of Unsteady Reacting Flow)

- Unsteady, compressible flow
- Finite volume method
- MUSCL scheme for convection
- Central-difference for diffusion
- Dynamically adaptive mesh refinement
  - Mesh size = $\Delta x_0 / 2^{Level}$, 10 levels
  - Finest mesh size: 1 micro-meter
- Point-implicit method for stiff ODEs
  - Time step ~ 0.4 nano-second



Chemical kinetics

- Chemical mechanisms for n-heptane (44 species) and DME (55, 113 species)
- These mechanisms well predict low-temperature ignition.

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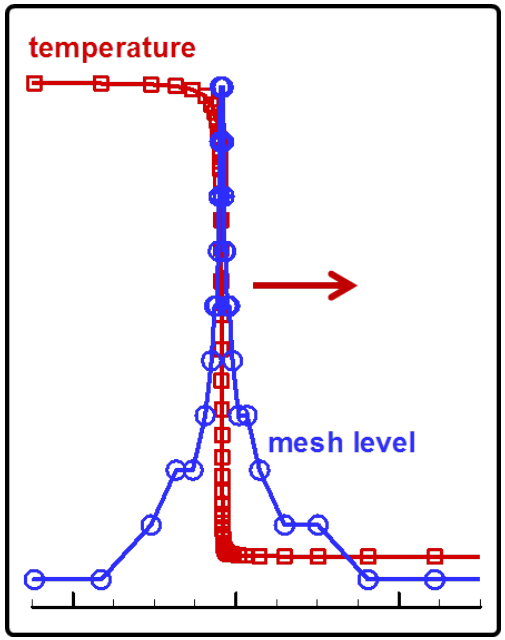

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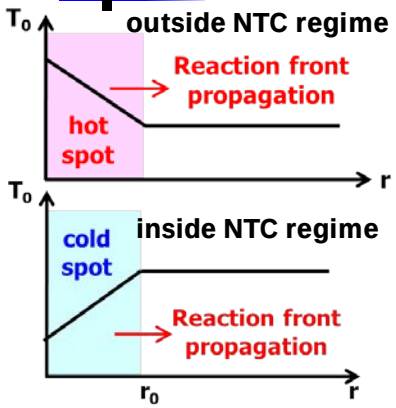
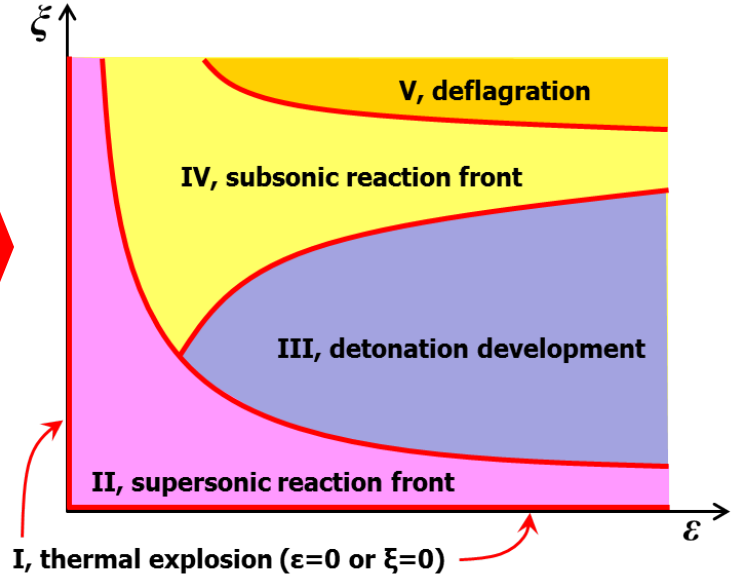
Different modes of reaction front propagation



$$\xi = \left(\frac{dT_0}{dr}\right) \Big/ \left(\frac{dT_0}{dr}\right)_c = a/u$$

$$\varepsilon = \frac{r_0}{a\tau_e}$$

Excitation time



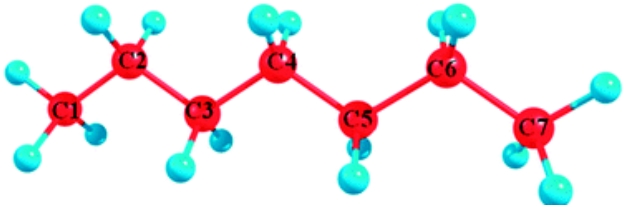
Different modes:

(Zeldovich 1980, Bartenev & Gelfand, 2000, Bradley 2002…)

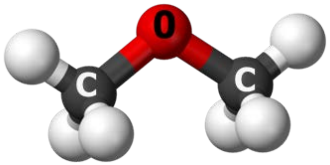
- I, Thermal explosion (homogeneous ignition): $u = \infty$ $(\nabla T = 0)$
- II, Supersonic reaction front: $u >> a >> S_u$ (small ∇T)
- III, Detonation development: $u \sim a >> S_u$
- IV, Subsonic reaction front: $a > u >> S_u$
- V, Deflagration / flame: $a >> u \sim Su$ (large ∇T)

Our work

- 2015PCI: autoignition and detonation from a cold spot, nC_7H_{16}
- 2015CNF: multi-stage heat release, nC_7H_{16}
- 2017PCI: different initial temperatures, CH_3OCH_3
- 2017PCI: concentration gradient, nC_7H_{16}
- 2019PCI: effects of NOx, CH_3OCH_3
- 2019CNF: fuel lean and CO_2 dilution, nC_7H_{16}



n-heptane, C_7H_{16}



DME, CH_3OCH_3

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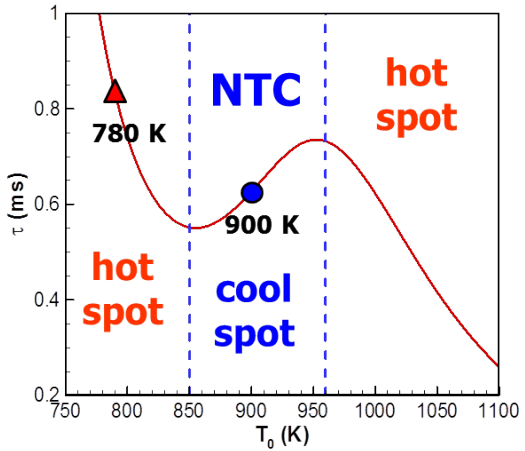

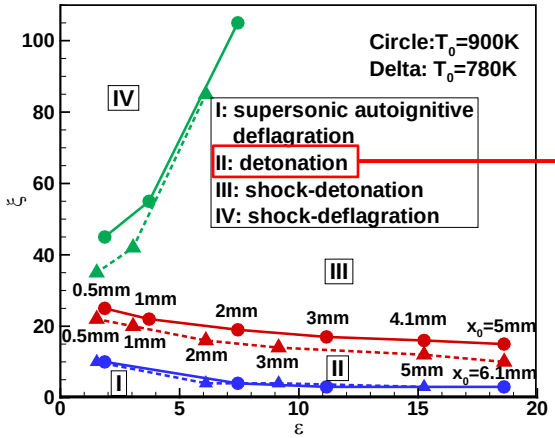

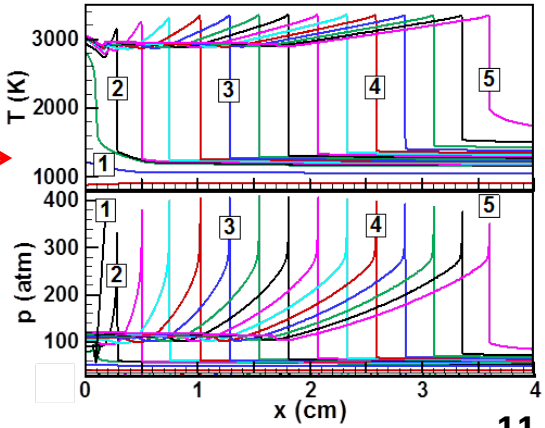

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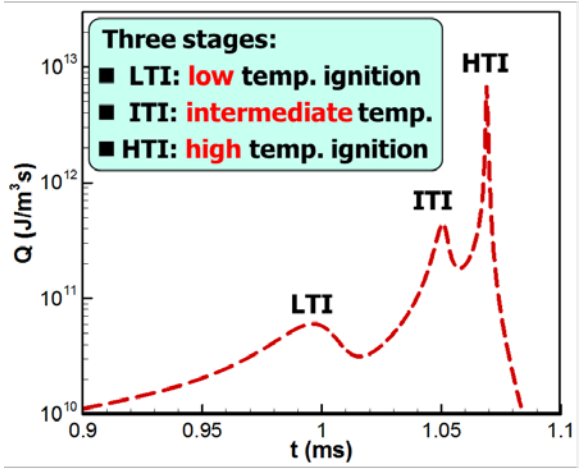

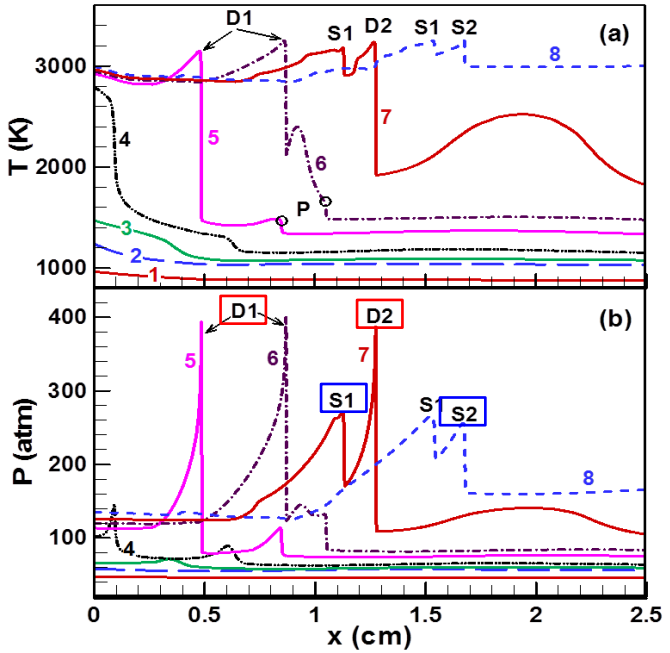

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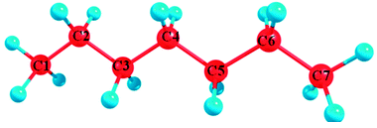

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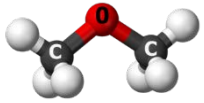
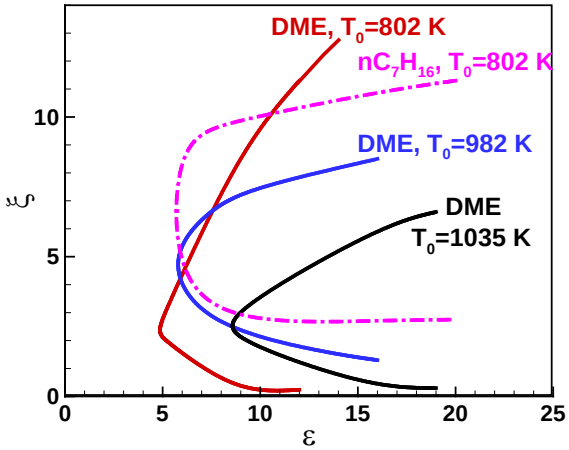
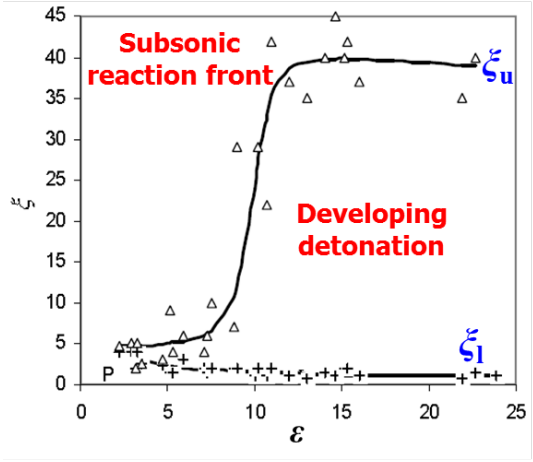


DME, CH_3OCH_3



(Bradley et al. 2002)



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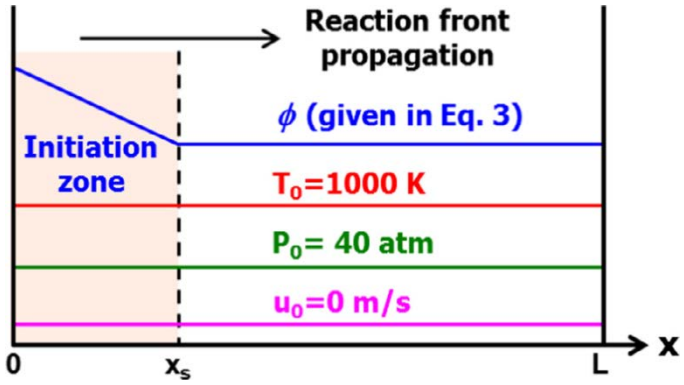

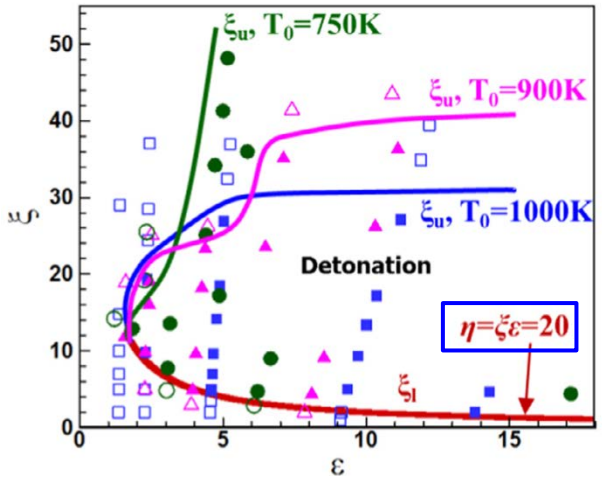

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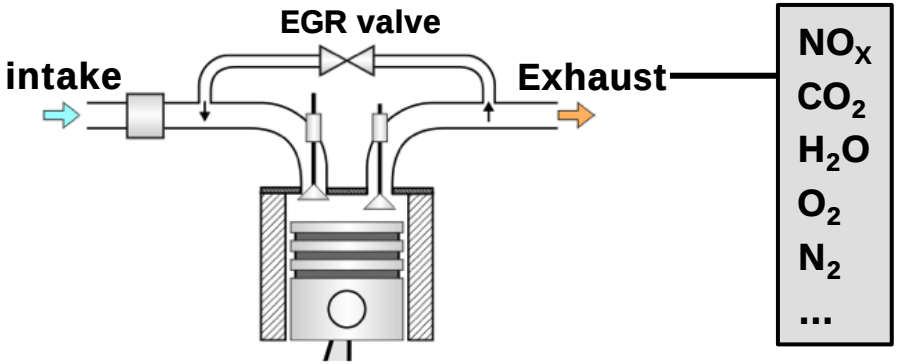
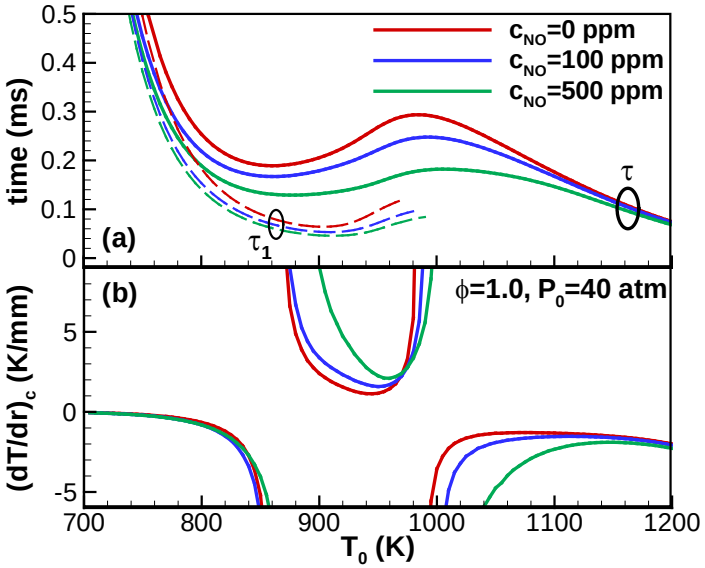
Effects of NOx addition

(Dai and Chen, 2019 PCI)

Exhaust gas recirculation (EGR)



$$\left(dc_{NO}/dr\right)_c = \left(a\left(d\tau/dc_{NO}\right)\right)^{-1}$$



- NO greatly promotes OH production and ignition
  - 1st stage: $HO_2+NO=NO_2+OH$, $DME+OH/H \rightarrow CH_3OCH_2 \rightarrow$ Low-T chemistry
  - 2nd stage: $NO_2+CH_3=NO+CH_3O$, $NO_2+H=NO+OH$, $HO_2+NO=NO_2+OH$
- Local NOx accumulation can induce autoignitive front propagation

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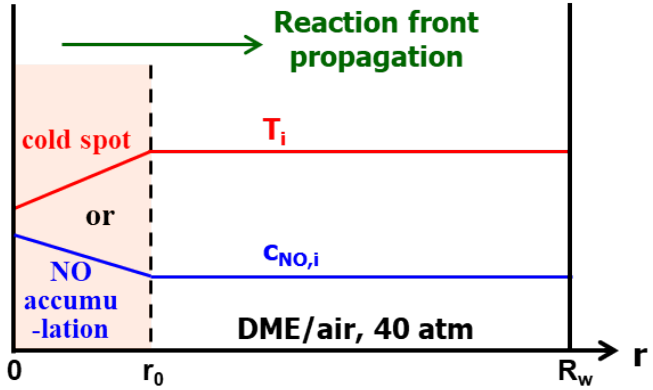

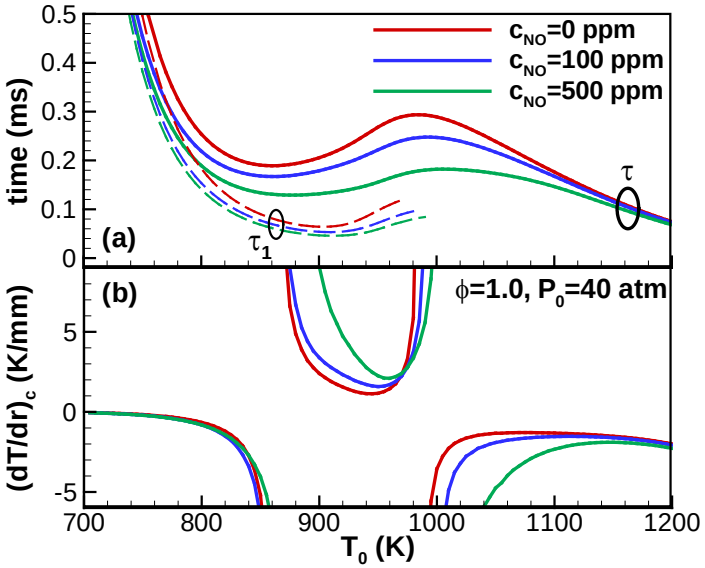

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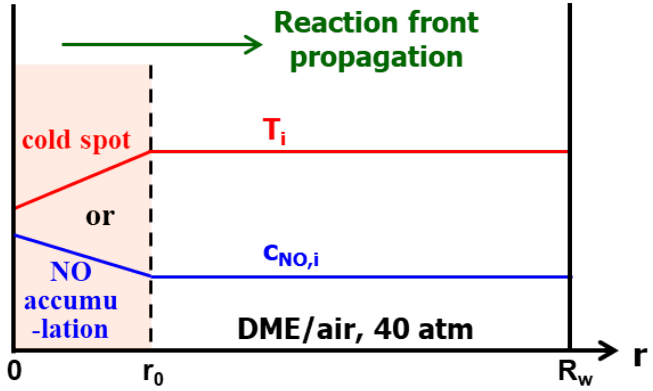

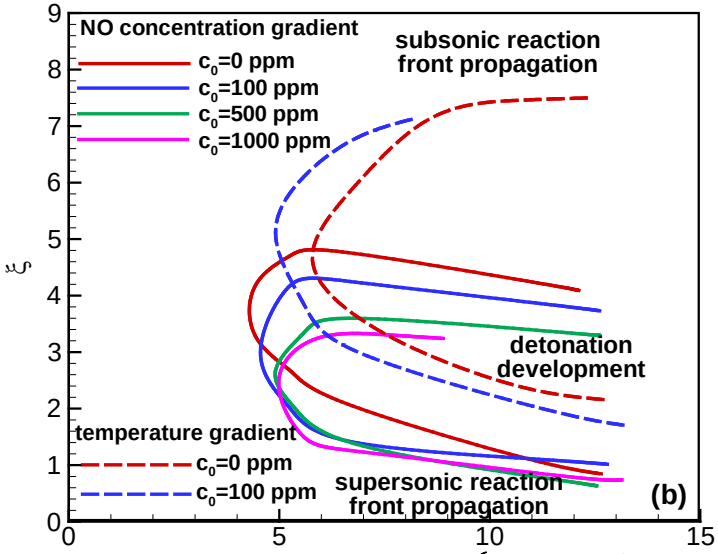

$$\xi = \frac{a}{u} = \begin{cases} (dT/dr)_i \,/\, (dT/dr)_{c,r_0/2} \\ (dc_{NO}/dr)_i \,/\, (dc_{NO}/dr)_{c,r_0/2} \end{cases}$$

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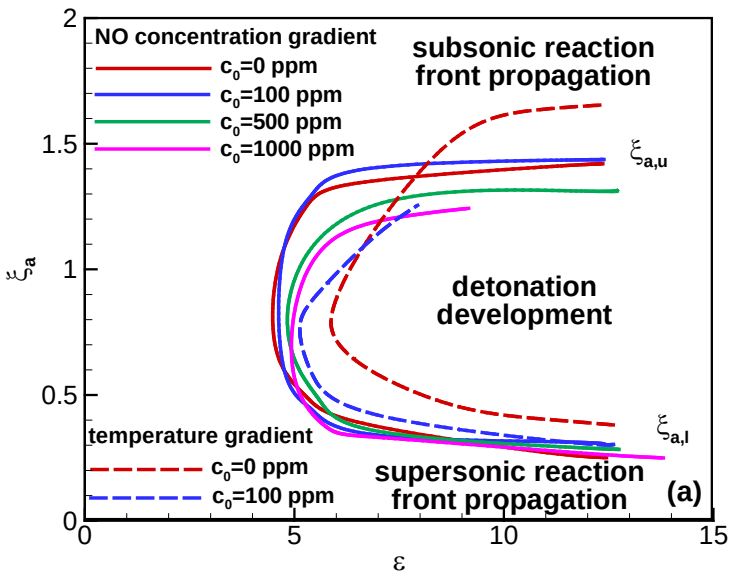
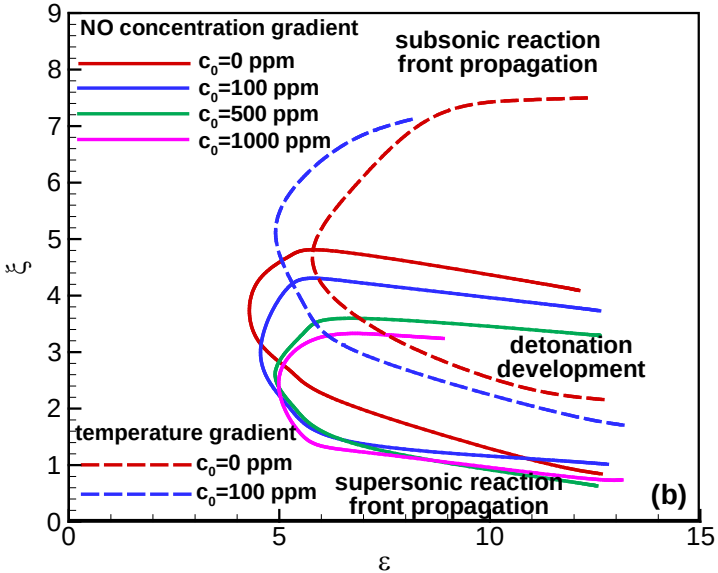




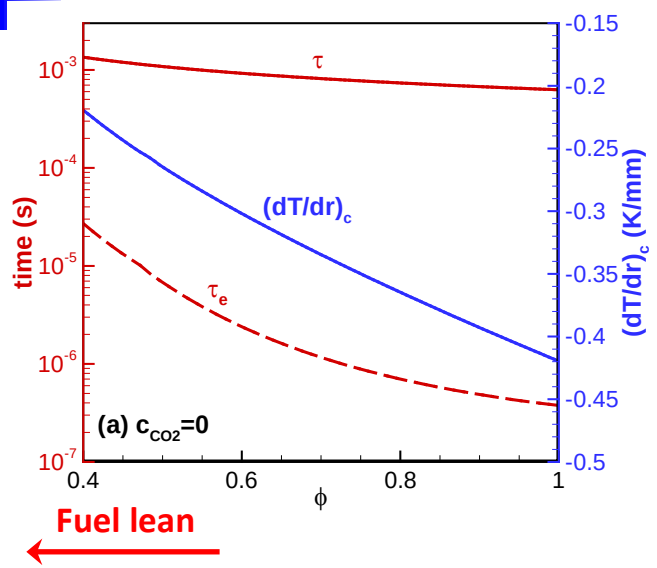
$$\xi_a = \frac{a_{r=r_0/2}}{S_{average}}$$

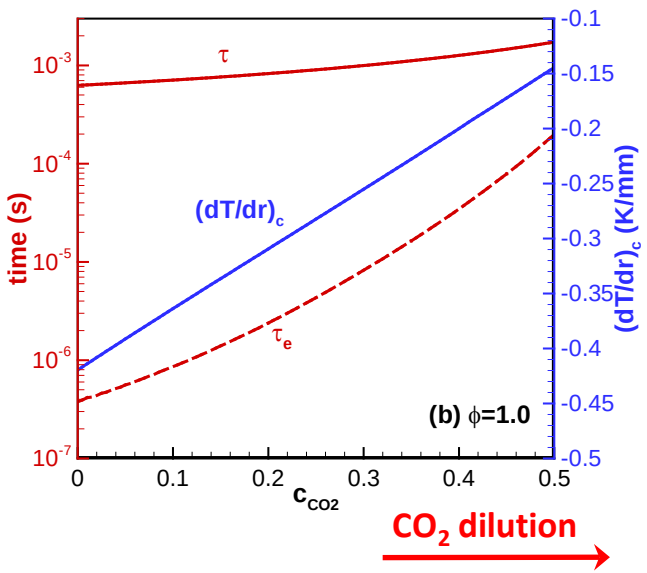
$$\xi = \frac{a}{u} = \begin{cases} (dT/dr)_i / (dT/dr)_{c,r_0/2} \\ (dc_{NO}/dr)_i / (dc_{NO}/dr)_{c,r_0/2} \end{cases}$$

- In ξ-ε diagram, detonation regime **strongly depends on** NO addition level and spot type (NO spot, cold spot)
- In ξ_a-ε diagram, detonation regimes **are close to each other**

Fuel lean or CO_2 dilution

(Dai, Chen, Gan, 2019 CNF)

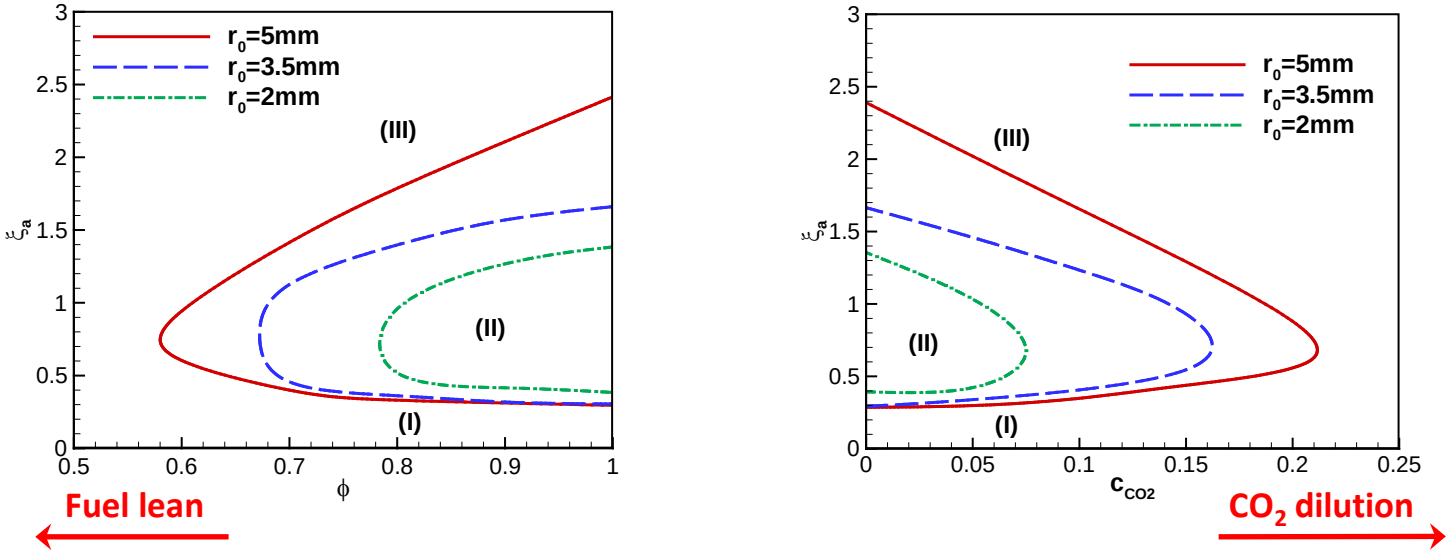




- Both τ and τ_e increase with decreasing ϕ or increasing c_{CO2}
- τ_e is much **more sensitive** and it can be enlarged by 100 times
- Heat release can be significantly **mitigated** by fuel lean or CO_2 dilution

Fuel lean or CO_2 dilution

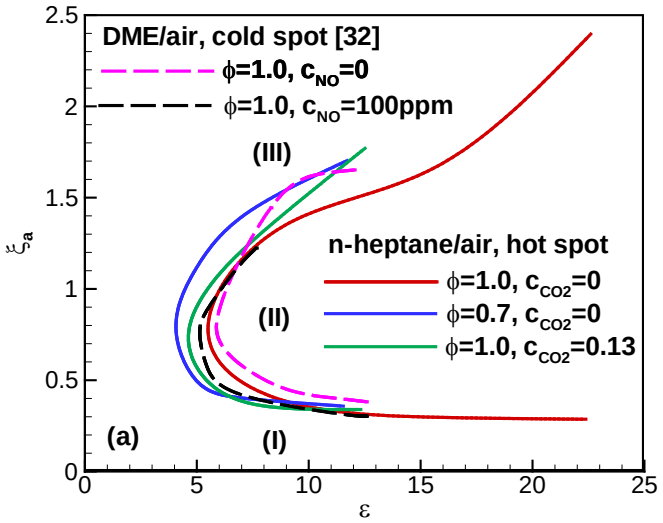
(Dai, Chen, Gan, 2019 CNF)



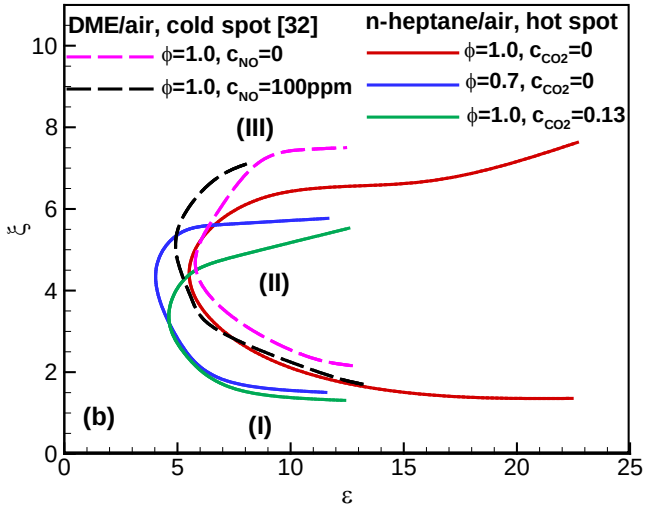
- (I) supersonic reaction front propagation, (II) detonation development, and (III) subsonic reaction front propagation
- Fuel lean or CO_2 dilution great reduces the propensity of detonation development

Fuel lean or CO_2 dilution

(Dai, Chen, Gan, 2019 CNF)



$$\xi_a = \frac{a_{r=r_0/2}}{S_{average}}$$



$$\xi = \left(\frac{dT_0}{dr}\right) \Big/ \left(\frac{dT_0}{dr}\right)_c = a/u$$

- In ξ-ε diagram, detonation regime strongly depends on equivalence ratio, NO addition and CO_2 dilution
- In ξ_a-ε diagram, detonation regimes are close to each other

Summary

- Detonation development regime depends on
  - fuel type
  - initial temperature / pressure / equivalence ratio / additives / dilution…
- Proper parameters to quantify detonation development regime ?

$$\xi = \left(\frac{dT_0}{dr}\right) \Big/ \left(\frac{dT_0}{dr}\right)_c = a/u, \quad \varepsilon = \frac{r_0}{a\tau_e}, \quad \xi\varepsilon = \frac{r_0 / u_a}{\tau_e}, \quad \xi_a = \frac{a_{r=r_0/2}}{S_{average}} \ldots ?$$

- Excitation time is an important parameter which is difficult to be measured in experiments or accurately predicted.
- Chemistry (Low-T chemistry, NOx) greatly affects the detonation development due to reactivity gradient

Acknowledgments

Natural Science Foundation of China

Thank you for your attention!