Direct Numerical Simulations of Multistage Ignition for a Stratified HCCI Engine with Exhaust Gas Recirculation : H_2O_2 Effect

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Mechanical and Aerospace Engineering

I-Motivation

- Fossil fuels depletion and EPA regulations drive the need for:
  - ❑ Alternative synthetic fuels
  - ❑ Efficient engines with high pressure compression ratios
  - ❑ Burning in the lean premixed mode to reduce emissions
- Homogenous Compression Charge Ignition (**HCCI**) Engines auto-ignite a homogenous lean premixed charge at high pressure compression ratios

III-Numerical Setup : HCCI

Volumetric heating compression at the TDC- P=30 atm T=834.5K (NTC) DME/Air mixture 55 species (Curran et al. CNF 1998)

Domain: 1.5x1.5 mm domain

362x362 grid points (4 μm mesh)

Fully compressible formulation

Periodic in all directions

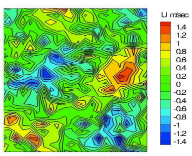
Stratification in T and ϕ using Pa[ssot–Pouquet] spectrum

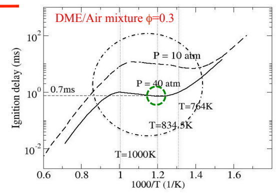
Uncorrelated T and ϕ spectrum

Re_λ=20

η= 5.3μm

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





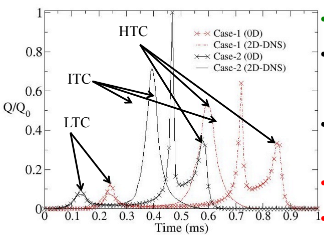
Initial H2O2 from EGR

Case-I	Case-II
Y_{H2O2}=0	Y_{H2O2}=400ppm

Initial spectrum conditions

	Mean	rms	Integral length Scale
U	0	0.5	1.24 mm
T	834.5 K	15K	1 mm
ϕ	0.3	0.1	1 mm

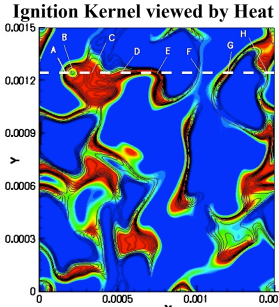
IV-NTC Autoignition (OD/DNS)

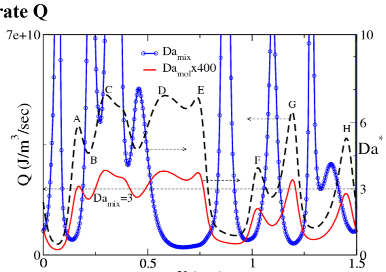


- **CONCLUSIONS-I**
- DME/Air has three NTC ignition stages
  - ❑ Low TC, Intermediate TC, High TC
- H_2O_2 from EGR enhances autoignition by increasing the OH radical pool
- 46% reduction in LTC ignition
- 34% reduction in HTC and ITC ignitions

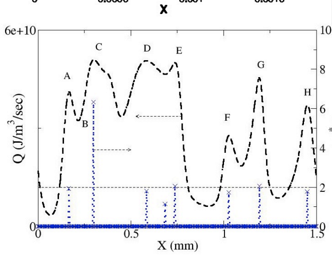
VI-Flame propgation Modes at LTC

Ignition Kernel viewed by Heat release rate Q

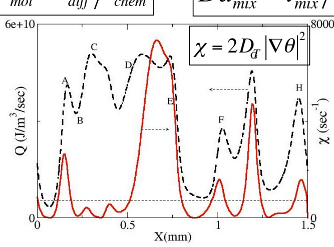




$$Da_{mol}=t_{diff}/t_{chem}$$ $$Da_{mix}=t_{mix}/t_{chem}$$



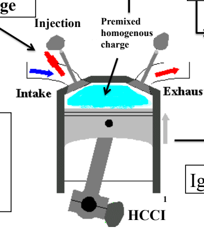
$$\chi=2D_T|\nabla\theta|^2$$



Deflagration wave at flame front A, D,E,F,G, and H

Homogeneous spontaneous ignition at point C

II-HCCI Operation and Challenges



Premixed ultra lean (ϕ< 0.45) homogeneous charge

High in-cylinder compression ratio

High efficiency (diesel engines)

Severe heat release

Low PM - Low NOx

Severe pressure rise and heat release

Low load : Low efficiency (HC-CO)

High load: limited by Heat release rate

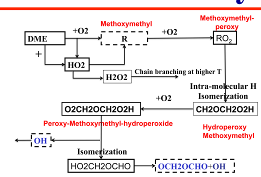
Ignition at low T < 1000 K

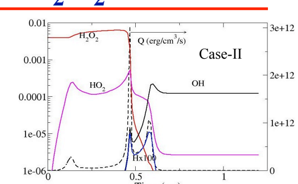
Detailed low temperature chemistry (LTC) models

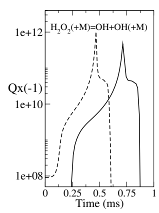
Not well understood (Objectives):

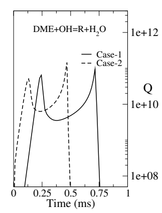
- **Autoignition at low temperature with thermal/mixture stratification**
- **Effect of exhaust gas recirculation (EGR) on autoignition**
- **The coupling effect of transport/chemistry on LTC ignition**

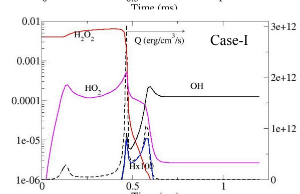
V-LTC chemistry and H_2O_2 Effect











$$t_{mix}=1/D_T|\nabla\theta|^2,\theta=(T-T_{min})/(T_{min}-T_{max})$$

$$t_{diff}=D_{IKI}/S_L^2$$

$$t_{chem}=\frac{C_{p,mix}T\rho}{Q}$$

$$D_{IKI}=D_{OH}+D_{HO_2}$$

$$S_D=\frac{\left(\omega_{IKI}-\frac{\partial}{\partial x_i}\left(D_{IKI}\rho\frac{\partial Y_{IKI}}{\partial x_i}\right)\right)}{\rho_u|\nabla Y_{IKI}|}$$

VII-Conclusion

- ❑ **DNSs are conducted for a stratified HCCI engine with EGR**
- ❑ **DME/air has three ignition stages in the NTC region initial conditions**
- ❑ **H_2O_2 addition from EGR accelerates ignition by the OH radical pool**
- ❑ **Thermal and mixture stratification introduce mixing time scales that interact strongly with chemistry after the LTC ignition stage**
- ❑ **Two different reaction front ignition modes are found : a homogeneous ignition and deflagration modes**
- ❑ **A criteria to distinguish between the different modes are developed based on the local time scales and radical pool**