Influence of low-temperature chemistry on steady detonations with curvature losses

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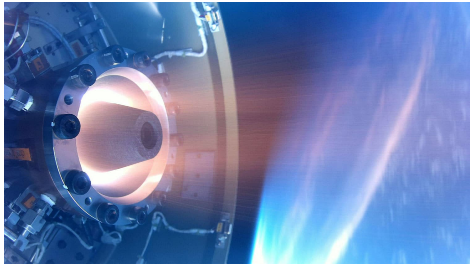
Motivation and objective

- Dimethyl ether (DME - CH_3OCH_3) is a promising alternative fuel
- Useful applications (ICE - RDE)
- Safety concerns in case of leaks
  - Oxygenated fuel more prone to ignition
  - Leaks in confined environments, which promotes DDT
- Low temperature chemistry (LTC) effect on detonations
  - Only few previous works
  - DDT run-up distance reduction
  - Smaller cell widths
  - LTC active at high levels of CO_2 dilution for ideal detonations

RENEWABLE DME®

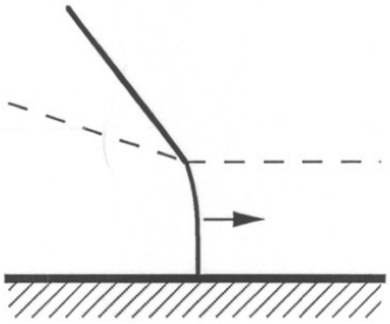
Image taken from Oberon Fuels.

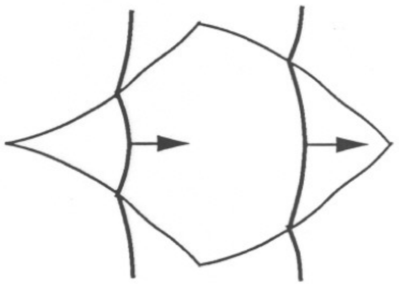


Motivation and **objective**

- Determine the **influence of LTC** on detonation velocity - curvature ($D - \kappa$) curves using DME as fuel

- Discuss **potential implications** on initiation, propagation and quenching of DME detonations





Pictures taken from Klein et al. report FM95-04

1D model including small curvature

Mathematical formulation

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho\frac{\left(\dot{\sigma} + wM^2\alpha\right)}{1 - M^2}$$

$$\frac{\mathrm{d}w}{\mathrm{d}t} = w\frac{(\dot{\sigma} - w\alpha)}{1 - M^2}$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\rho w^2\frac{(\dot{\sigma} - w\alpha)}{1 - M^2}$$

$$\frac{\mathrm{d}Y_k}{\mathrm{d}t} = \frac{W_k\dot{\omega}_k}{\rho}, \quad \left(k = 1, \ldots, N\right)$$

$$\dot{\sigma} = \sum_{k=1}^{N}\left(\frac{\overline{W}}{W_k} - \frac{h_k}{c_pT}\right)\frac{\mathrm{d}Y_k}{\mathrm{d}t}$$ Thermicity

$$\alpha = \frac{1}{A}\frac{\mathrm{d}A}{\mathrm{d}x} = \kappa\left(\frac{D}{w} - 1\right)$$ Detonation curvature term

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$$T_o = 300\ \mathrm{K}\ ; p_o = 100\ \mathrm{kPa}$$

$$\mathrm{CH_3OCH_3 + 3O_2} + X\mathrm{CO_2}$$

Two detailed chemistry mechanisms

39 species & 154 reactions (+21 for LTC: R155-R175)

No Low Temperature Chemistry (No LTC)

Low Temperature Chemistry (LTC)

Bhagatwala et al. PROCI, vol. 35, no. 2, pp. 1157-1166, 2015

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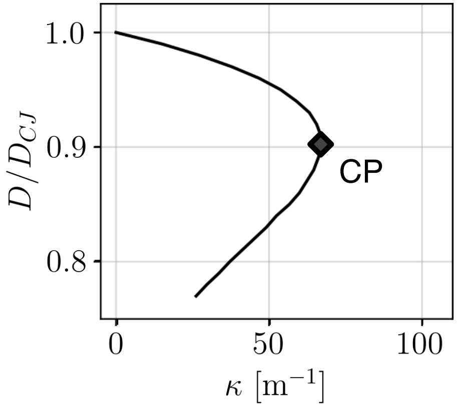

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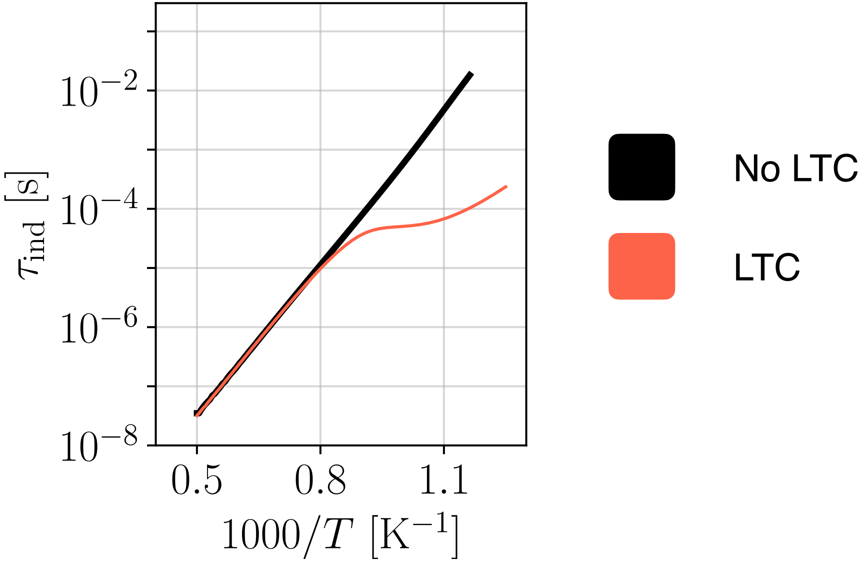
Results

Influence of LTC: D-kappa curves - $CH_3OCH_3 + 3\ O_2 + 0\ CO_2$

Induction time vs. $1000/T$



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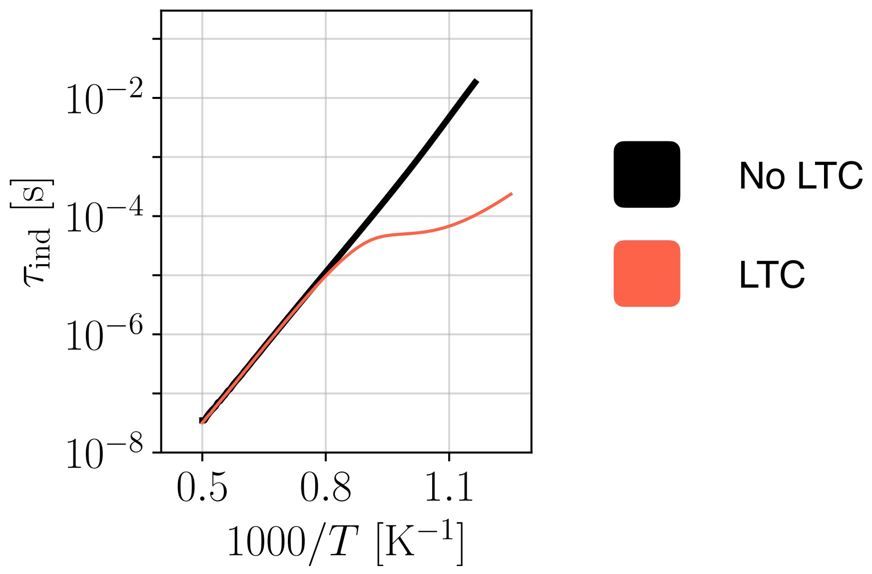
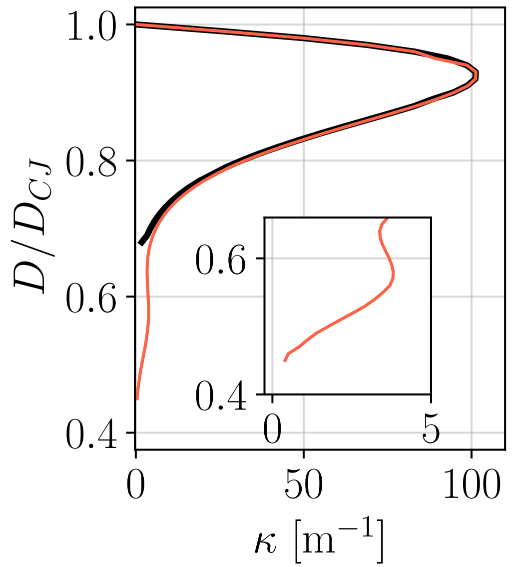


Detonation speed vs. curvature



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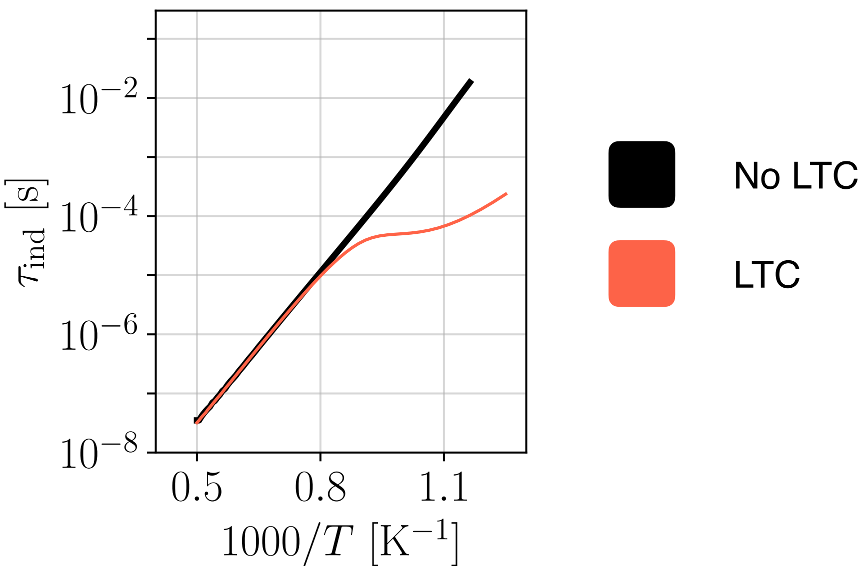

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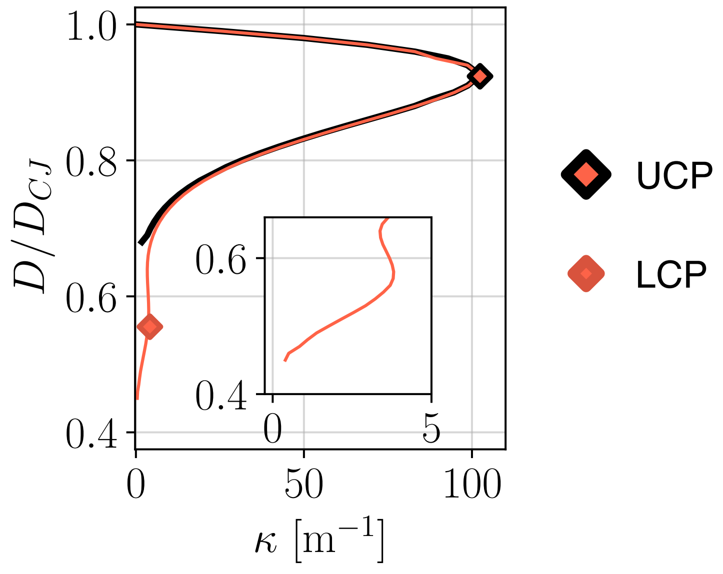
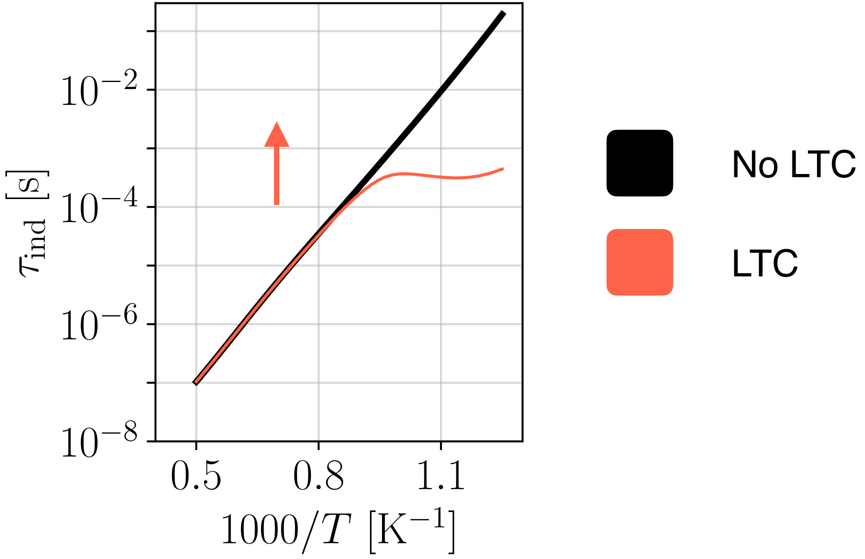


Existence of a lower critical point with LTC

Results

Influence of LTC: D-kappa curves - $CH_3OCH_3 + 3\ O_2 +$ **6** CO_2

Induction time vs. $1000/T$



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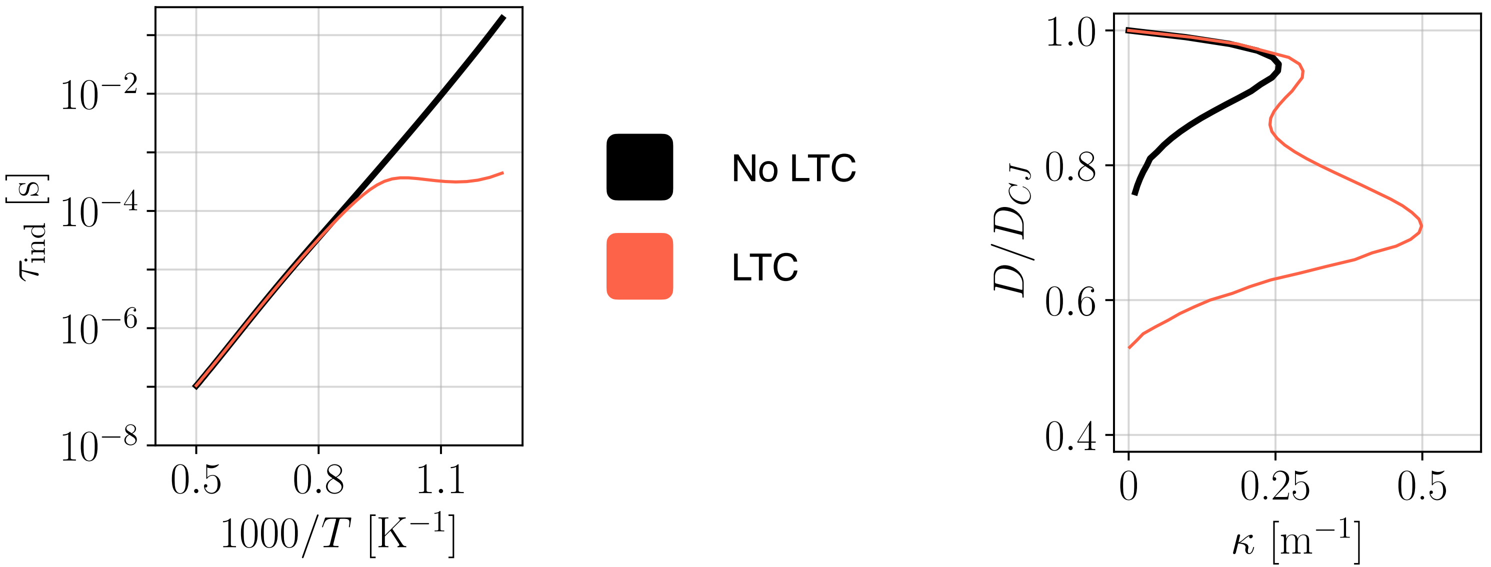

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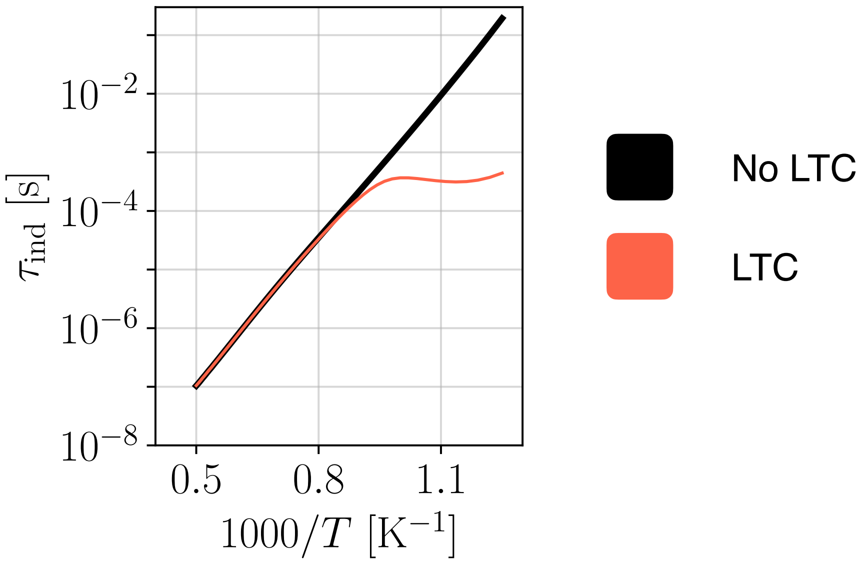
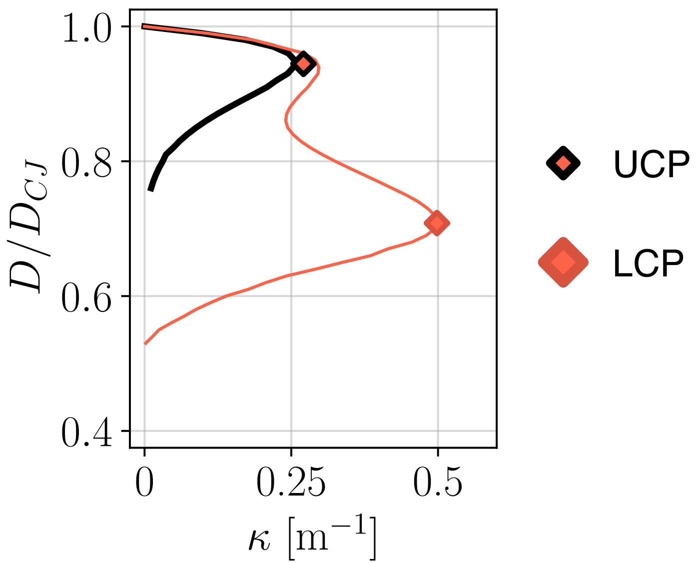


Detonation speed vs. curvature



LCP shifted towards higher curvatures with increasing CO_2 addition

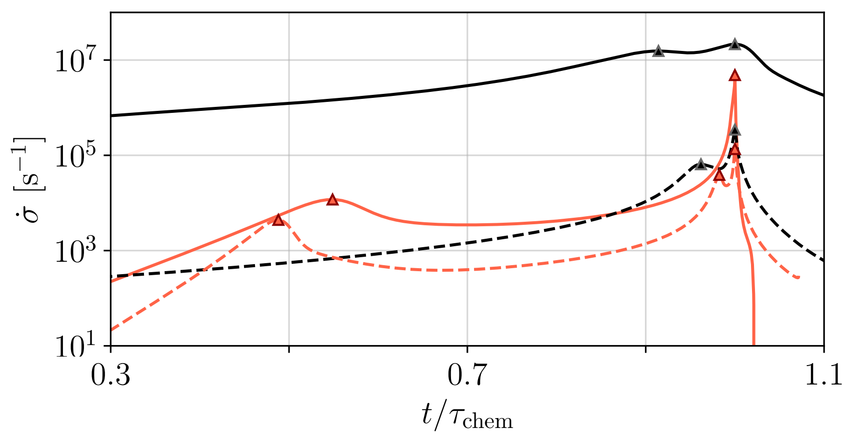
Results

Influence of LTC: Thermochemical analysis - CH_3OCH_3 + 3 O_2 + **X** CO_2

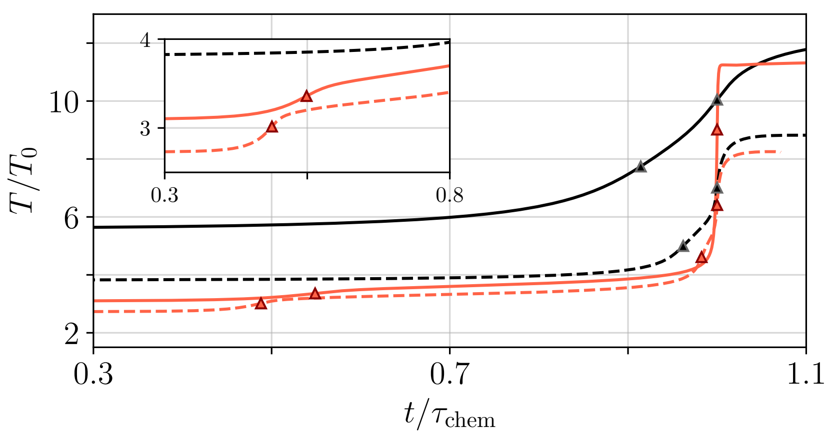
$0CO_2$, UCP — $6CO_2$, UCP

$0CO_2$, LCP — $6CO_2$, LCP

Thermicity profiles



Temperature profiles



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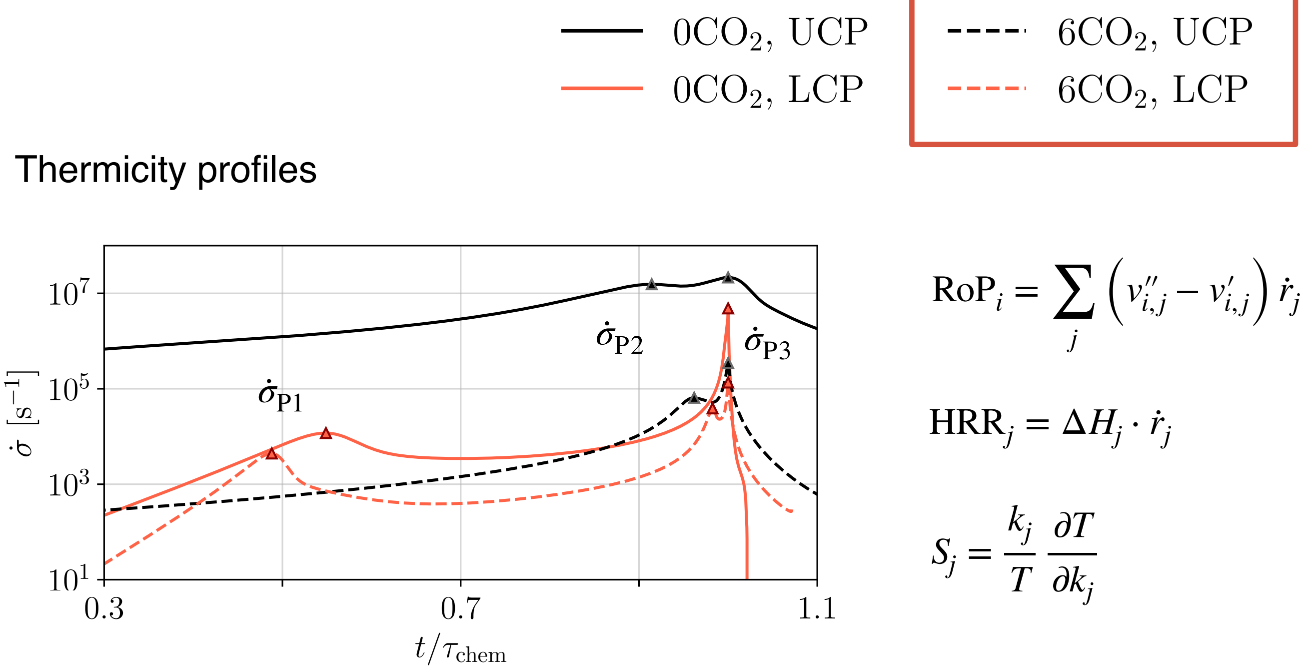

Thermicity profiles

$$\mathrm{RoP}_i = \sum_j \left(\nu''_{i,j} - \nu'_{i,j}\right) \dot{r}_j$$

Rate of production

$$\mathrm{HRR}_j = \Delta H_j \cdot \dot{r}_j$$

Heat release rate

$$S_j = \frac{k_j}{T} \frac{\partial T}{\partial k_j}$$

Sensitivity of reaction rate on temperature

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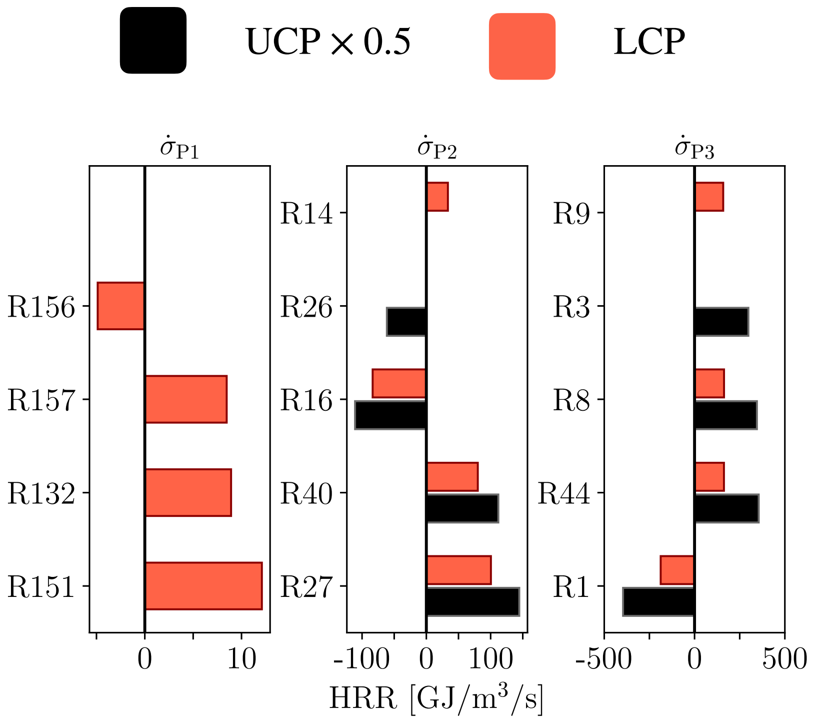


DME Heat release rate

$$\mathrm{HRR}_j = \Delta H_j \cdot \dot{r}_j$$

R1: $H + O_2 = O + OH$

R3: $H_2 + OH = H + H_2O$

R8: $H + OH + M = H_2O + M$

R9: $H + O_2(+M) = HO_2(+M)$

R14: $2HO_2 = H_2O_2 + O_2$

R16: $H_2O_2(+M) = 2OH(+M)$

R26: $HCO + M = CO + H + M$

R27: $HCO + O_2 = CO + HO_2$

R40: $CH_2O + OH = H_2O + HCO$

R44: $CH_3 + O = CH_2O + H$

R132: $CH_3OCH_3 + OH = CH_3OCH_2 + H_2O$

R151: $CH_3OCH_2 + O_2 = CH_3OCH_2O_2$

R156: $CH_3OCH_2O_2 = CH_2OCH_2O_2H$

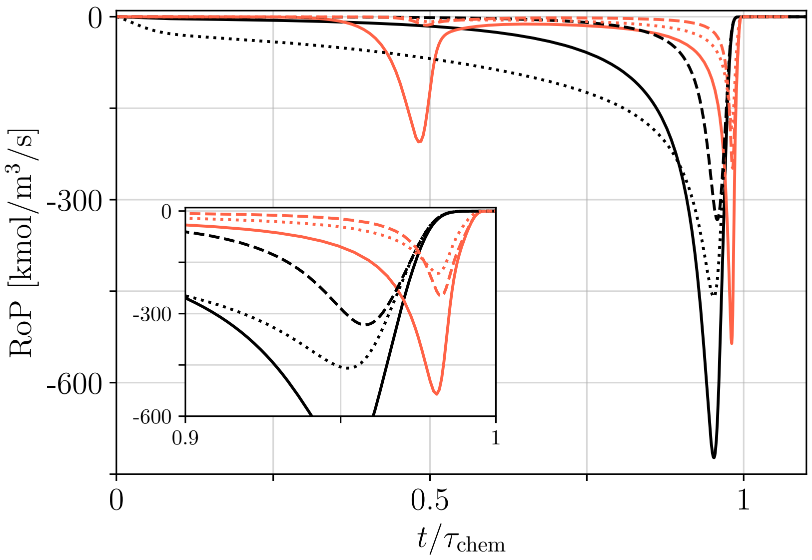
R157: $CH_2OCH_2O_2H = 2CH_2O + OH$

LTC

Results

Influence of LTC: Thermochemical analysis - CH_3OCH_3 + 3 O_2 + **6** CO_2

UCP   LCP × 2



DME Rate of production

$$\mathrm{RoP_{DME}} = \sum_j \left(v''_{i,j} - v'_{i,j}\right) \dot{r}_j$$

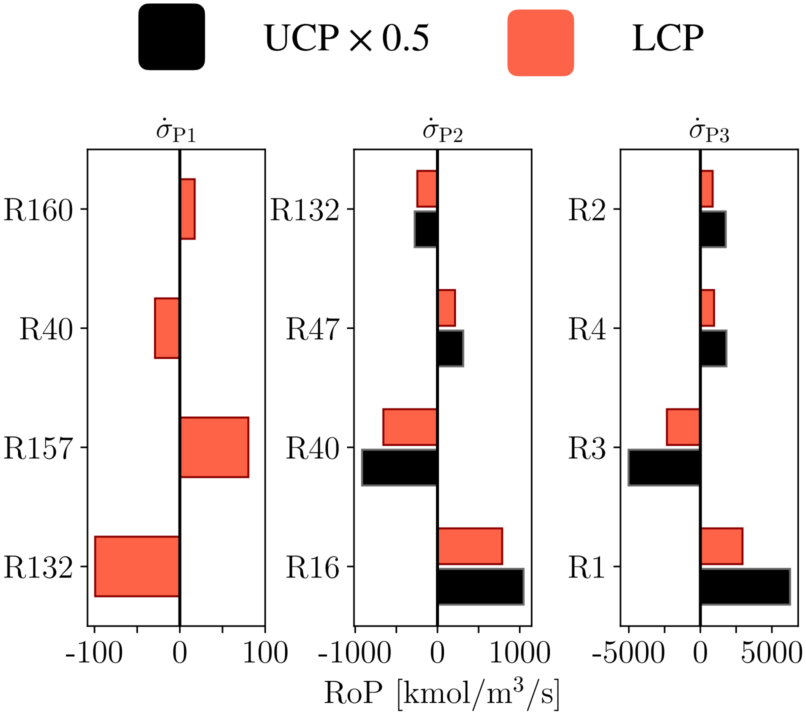
R132: $CH_3OCH_3 + OH = CH_3OCH_2 + H_2O$ (solid line)

R133: $CH_3OCH_3 + H = CH_3OCH_2 + H_2$ (dashed line)

R134: $CH_3 + CH_3OCH_3 = CH_3OCH_2 + CH_4$ (dotted line)

Results

Influence of LTC: Thermochemical analysis - CH_3OCH_3 + 3 O_2 + **6** CO_2



OH Rate of production

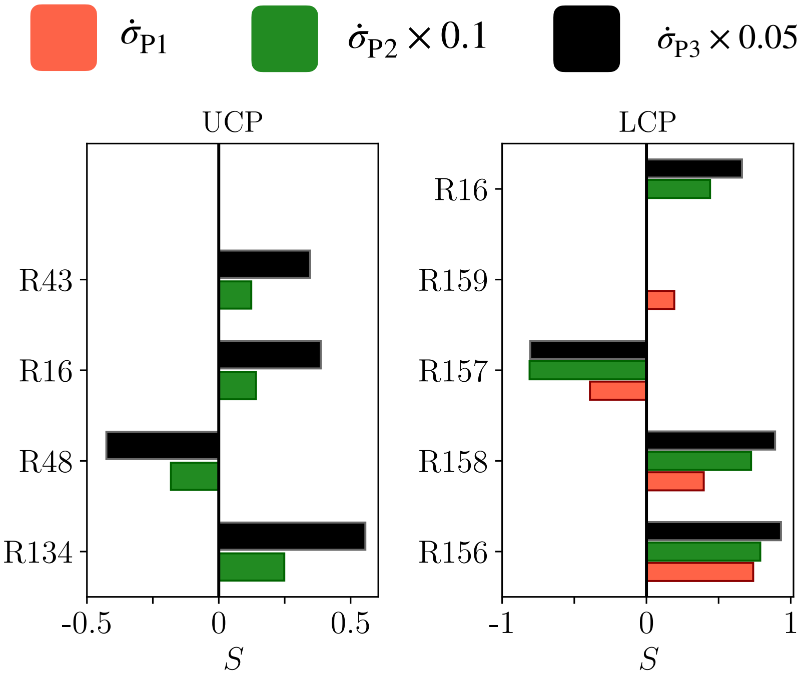
$$\mathrm{RoP}_{\mathrm{OH}} = \sum_j \left(v''_{i,j} - v'_{i,j}\right) \dot{r}_j$$

R1: $H + O_2 = O + OH$
R2: $H_2 + O = H + OH$
R3: $H_2 + OH = H + H_2O$
R4: $H_2O + O = 2OH$
R16: $H_2O_2(+M) = 2OH(+M)$
R40: $CH_2O + OH = H_2O + HCO$
R47: $CH_3 + HO_2 = CH_3O + OH$
R132: $CH_3OCH_3 + OH = CH_3OCH_2 + H_2O$
R157: $CH_2OCH_2O_2H = 2CH_2O + OH$
R160: $HO_2CH_2OCHO = OCH_2OCHO + OH$

LTC

Results

Influence of LTC: Thermochemical analysis - $CH_3OCH_3 + 3\ O_2 +$ **6** CO_2



Sensitivity of reaction rate on temperature

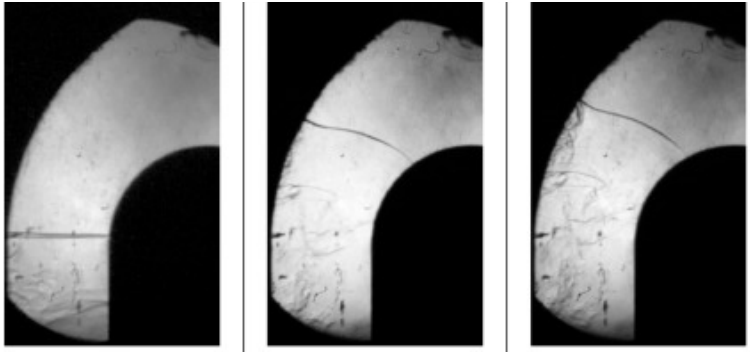
$$S_j = \frac{k_j}{T} \frac{\partial T}{\partial k_j}$$

R16: $H_2O_2(+M) = 2OH(+M)$
R43: $CH_2O + CH_3 = CH_4 + HCO$
R48: $2CH_3(+M) = C_2H_6(+M)$
R134: $CH_3 + CH_3OCH_3 = CH_3OCH_2 + CH_4$
R156: $CH_3OCH_2O_2 = CH_2OCH_2O_2H$
R157: CH2OCH2O2H = $2CH_2O + OH$
R158: $CH_2OCH_2O_2H + O_2 = O_2CH_2OCH_2O_2H$
R159: $O_2CH_2OCH_2O_2H = HO_2CH_2OCHO + OH$

LTC

Potential implications

- Effect of LCP on detonations propagating in tubes/transmission to open space is not straightforward
    - Potential changes in the cellular structure
    - Non-trivial re-initiation dynamics
- Influence on galloping detonations
    - Change in frequency
    - Promote re-initiation
- Increase of the detonability envelope as in flammability for DME
- Improved efficiency of pre-detonators in PDE
- Detonation initiation in ICE



Pictures taken from Josué Melguizo-Gavilanes et al. CNF 223, 2021

Conclusions and future efforts

- Existence of a second critical point (LCP) only when LTC is considered
- Shift on criticality from small to large velocity deficits
- LTC enables an increased resistance to curvature-induced losses in the low velocity regime
- The production of OH and increase in temperature during early stages (LTC) is crucial to activate the main heat release stage (HTC)

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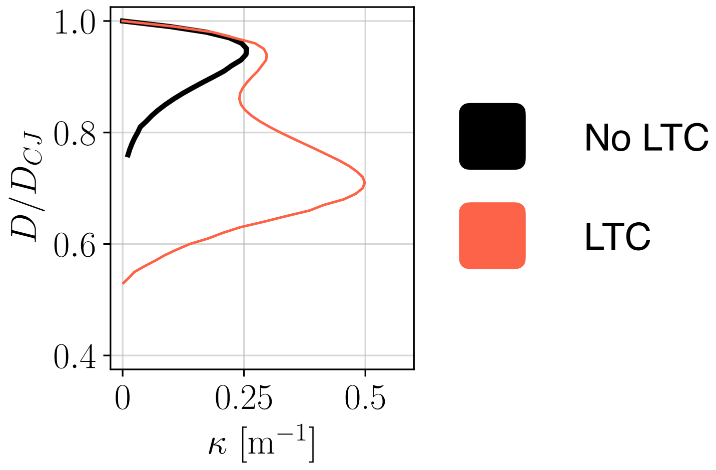
Explore the influence of LTC via:

- Simulations
  - Detonation-inert layer interaction
- Experiments
  - Transition to open space
  - Curved geometries

FVL and JMG acknowledge the financial support from Agence National de la Rechercher Program JCJC (FASTD ANR-20-CE05-0011-01)



Thank you for your attention!