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

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Motivation and objective

- Dimethyl ether (DME - CH$_3$OCH$_3$) 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
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

\[
\frac{d\rho}{dt} = -\rho \frac{(\dot{\sigma} + wM^2\alpha)}{1 - M^2}
\]

\[
\frac{dw}{dt} = w \frac{(\dot{\sigma} - w\alpha)}{1 - M^2}
\]

\[
\frac{dp}{dt} = -\rho w^2 \frac{(\dot{\sigma} - w\alpha)}{1 - M^2}
\]

\[
\frac{dY_k}{dt} = \frac{W_k \dot{\omega}_k}{\rho}, \quad (k = 1, \ldots, N)
\]

\[
\dot{\sigma} = \sum_{k=1}^{N} \left( \frac{W}{W_k} - \frac{h_k}{c_p T} \right) \frac{dY_k}{dt}
\]

Thermicity

\[
\alpha = \frac{1}{A} \frac{dA}{dx} = \kappa \left( \frac{D}{w} - 1 \right)
\]

Detonation curvature term
1D model including small curvature

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Detonation curvature term

\[ T_o = 300 \text{ K}; p_o = 100 \text{ kPa} \]

\[ \text{CH}_3\text{OCH}_3 + 3\text{O}_2 + \text{XCO}_2 \]

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
1D model including small curvature

Mathematical formulation

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Results

Influence of LTC: D-kappa curves - CH₃OCH₃ + 3 O₂ + 0 CO₂

Induction time vs. 1000/T

- No LTC
- LTC
Results

Influence of LTC: D-kappa curves - CH$_3$OCH$_3$ + 3 O$_2$ + 0 CO$_2$

Induction time vs. $1000/T$

Detonation speed vs. curvature

- $\tau_{\text{ind}}$ [s] vs. $1000/T$ [K$^{-1}$]
- $D/D_{\text{ref}}$ vs. $\kappa$ [m$^{-1}$]

Mixture: DME + 3 O$_2$ + 0 CO$_2$
Results

Influence of LTC: D-kappa curves - CH$_3$OCH$_3$ + 3 O$_2$ + 0 CO$_2$

Induction time vs. $1000/T$

Detonation speed vs. curvature

Existence of a lower critical point with LTC
Results

Influence of LTC: D-kappa curves - CH$_3$OCH$_3$ + 3 O$_2$ + 6 CO$_2$

Induction time vs. 1000/\(T\)

\[
\bar{\tau}_{\text{ind}} \quad [s]
\]

\[
1000/T \quad [K^{-1}]
\]

- No LTC
- LTC
Results

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Induction time vs. $1000/T$

Detonation speed vs. curvature

\[ \tau_{\text{ind}} [s] \]

\[ D/D_{\text{CJ}} \]

Mixture: DME + 3 O$_2$ + 6 CO$_2$
Results

Influence of LTC: D-kappa curves - CH$_3$OCH$_3$ + 3 O$_2$ + 6 CO$_2$

Induction time vs. $1000/T$

Detonation speed vs. curvature

LCP shifted towards higher curvatures with increasing CO$_2$ addition
Results

Influence of LTC: Thermochemical analysis - $\text{CH}_3\text{OCH}_3 + 3 \text{ O}_2 + X \text{ CO}_2$

Thermicity profiles

Temperature profiles
Results
Influence of LTC: Thermochemical analysis - CH\(_3\)OCH\(_3\) + 3 O\(_2\) + 6 CO\(_2\)

Thermicity profiles

\[ \text{RoP}_i = \sum_j \left( v''_{i,j} - v'_{i,j} \right) \dot{r}_j \]  
Rate of production

\[ \text{HRR}_j = \Delta H_j \cdot \dot{r}_j \]  
Heat release rate

\[ S_j = \frac{k_j}{T} \frac{\partial T}{\partial k_j} \]  
Sensitivity of reaction rate on temperature
Results

Influence of LTC: Thermochemical analysis - CH₃OCH₃ + 3 O₂ + 6 CO₂

DME Heat release rate

\[ \text{HRR}_j = \Delta H_j \cdot \dot{r}_j \]

- \( \dot{r}_1 \): H + O₂ → O + OH
- \( \dot{r}_3 \): H₂ + OH → H + H₂O
- \( \dot{r}_8 \): H + OH + M → H₂O + M
- \( \dot{r}_9 \): H + O₂(±M) → HO₂(±M)
- \( \dot{r}_{14} \): 2HO₂ → H₂O₂ + O₂
- \( \dot{r}_{16} \): H₂O₂(±M) → 2OH(±M)
- \( \dot{r}_{26} \): HCO + M → CO + H + M
- \( \dot{r}_{27} \): HCO + O₂ → CO + HO₂
- \( \dot{r}_{40} \): CH₂O + OH → H₂O + HCO
- \( \dot{r}_{44} \): CH₃ + O → CH₂O + H
- \( \dot{r}_{132} \): CH₃OCH₃ + OH → CH₃OCH₂ + H₂O
- \( \dot{r}_{151} \): CH₃OCH₂ + O₂ → CH₃OCH₂O₂
- \( \dot{r}_{156} \): CH₃OCH₂O₂ → CH₃OCH₂O₂H
- \( \dot{r}_{157} \): CH₂OCH₂O₂H → 2CH₂O + OH

UCP × 0.5  LCP
Results

Influence of LTC: Thermochemical analysis - \( \text{CH}_3\text{OCH}_3 + 3 \text{O}_2 + 6 \text{CO}_2 \)

\[
\text{DME Rate of production}
\]

\[
\text{RoP}_{\text{DME}} = \sum_j \left( v''_{i,j} - v'_{i,j} \right) \dot{r}_j
\]

R132: \( \text{CH}_3\text{OCH}_3 + \text{OH} = \text{CH}_3\text{OCH}_2 + \text{H}_2\text{O} \)
R133: \( \text{CH}_3\text{OCH}_3 + \text{H} = \text{CH}_3\text{OCH}_2 + \text{H}_2 \)
R134: \( \text{CH}_3 + \text{CH}_3\text{OCH}_3 = \text{CH}_3\text{OCH}_2 + \text{CH}_4 \)
Results

Influence of LTC: Thermochemical analysis - CH$_3$OCH$_3$ + 3 O$_2$ + 6 CO$_2$

\[ \text{OH Rate of production} \]

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

- \( \text{R1: } \text{H} + \text{O}_2 = \text{O} + \text{OH} \)
- \( \text{R2: } \text{H}_2 + \text{O} = \text{H} + \text{OH} \)
- \( \text{R3: } \text{H}_2 + \text{OH} = \text{H} + \text{H}_2\text{O} \)
- \( \text{R4: } \text{H}_2\text{O} + \text{O} = 2\text{OH} \)
- \( \text{R16: } \text{H}_2\text{O}_2(+\text{M}) = 2\text{OH}(+\text{M}) \)
- \( \text{R40: } \text{CH}_2\text{O} + \text{OH} = \text{H}_2\text{O} + \text{HCO} \)
- \( \text{R47: } \text{CH}_3 + \text{HO}_2 = \text{CH}_3\text{O} + \text{OH} \)
- \( \text{R132: } \text{CH}_3\text{OCH}_3 + \text{OH} = \text{CH}_3\text{OCH}_2 + \text{H}_2\text{O} \)
- \( \text{R157: } \text{CH}_2\text{OCH}_2\text{O}_2\text{H} = 2\text{CH}_2\text{O} + \text{OH} \)
- \( \text{R160: } \text{HO}_2\text{CH}_2\text{OCHO} = \text{OCH}_2\text{OCHO} + \text{OH} \)
Results
Influence of LTC: Thermochemical analysis - CH₃OCH₃ + 3 O₂ + 6 CO₂

Sensitivity of reaction rate on temperature

\[ S_j = \frac{k_j}{T} \frac{\partial T}{\partial k_j} \]

\( R16: \ H₂O₂(+M) = 2OH(+M) \)
\( R43: \ CH₂O + CH₃ = CH₄ + HCO \)
\( R48: \ 2CH₃(+M) = C₂H₆(+M) \)
\( R134: \ CH₃ + CH₃OCH₃ = CH₃OCH₂ + CH₄ \)
\( R156: \ CH₃OCH₂O₂ = CH₂OCH₂O₂H \)
\( R157: \ CH₂OCH₂O₂H = 2CH₂O + OH \)
\( R158: \ CH₂OCH₂O₂H + O₂ = O₂CH₂OCH₂O₂H \)
\( R159: \ O₂CH₂OCH₂O₂H = HO₂CH₂OCHO + OH \)
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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- Existence of a second critical point (LCP) only when LTC is considered
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Explore the influence of LTC via:
- Simulations
  - Detonation-inert layer interaction
- Experiments
  - Transition to open space
  - Curved geometries
Thank you for your attention!