A methodology to develop simplified kinetic schemes for detonations simulations

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● Motivation and objective
● 1D Model
● 1D Results
● 2D Results
● Conclusions and future efforts

Numerical soot-foil obtained with stoichiometric H₂-O₂ detonation
Motivation and objective

- Modeling chemistry is still a challenge
- Flames: Several approaches
  - Efforts because of industrial needs (turbulent combustion)
  - Huge detailed mechanisms for HC (~100 species; ~1000 reactions)
  - Improved reduction techniques
- Detonations: usually single-step Arrhenius
  - Fair qualitative agreement
  - Lack for quantitative predictions (initiation, quenching)
  - Conventional 0D (induction time) or 1D (ideal ZND) fitting procedures
Motivation and objective

- Propose a new fitting procedure for reduced chemical mechanisms for stoichiometric hydrogen-oxygen detonations
  - Steady 1D curved ($\kappa$) detonations
  - Matching the predicted critical curvatures ($\kappa_{\text{crit}}$)
  - Predictive reduced chemistry

- Check the implications on multi-dimensional simulations

Pictures taken from Klein et al. report FM95-04
1D model including small curvature

Mathematical formulation

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

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

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

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

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

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

Thermicity

Detonation curvature term
1D model including small curvature

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Detonation curvature term

\[
T_o = 300 \text{ K}; p_o = 100 \text{ kPa}; \quad 2\text{H}_2 + \text{O}_2
\]

Single step chemistry

\[
F \rightarrow P \quad k_T = k \exp \left( -\frac{E_a}{R_u T} \right)
\]

Three step chemistry

Initiation \quad F \rightarrow Y \quad k_I = k_C \exp \left[ -\frac{E_I}{R_u \left( \frac{1}{T_I} - \frac{1}{T} \right)} \right]

Branching \quad F + Y \rightarrow 2Y \quad k_B = k_C \exp \left[ -\frac{E_B}{R_u \left( \frac{1}{T_B} - \frac{1}{T} \right)} \right]

Termination \quad Y \rightarrow P \quad k_T = k_C
1D model including small curvature

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Termination \( Y \rightarrow P \) \( k_T = k_C \)
1D Results
Chemistry: standard 0D fitting with induction time - D-kappa curves

**Induction time vs. 1000/T**

- Mevel et al.
- Ref. 1-step
- Ref. 3-step

**Chemical parameters**

**Single step chemistry**

- $k = 1.1 \times 10^9 \text{ s}^{-1}$
- $E_a/R_u = 11277 \text{ K}$

**Three step chemistry**

- $k_C = 2 \times 10^7 \text{ s}^{-1}$
- $E_I/R_u = 25000 \text{ K}$
- $E_B/R_u = 9300 \text{ K}$
- $T_I = 2431 \text{ K}$
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- Chapman-Jouguet conditions do not match
- Thermicity profiles are smoother with simplified mechanisms
1D Results

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Detonation speed vs. curvature

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- $\kappa_{crit}$ [m$^{-1}$] 67.4 74.8 168.5 This study
- $1/h_{crit}$ [m$^{-1}$] 41.7 50 166.7 Reference

1D Results

Influence of the fitting parameters

Single step chemistry
1D Results

Influence of the fitting parameters

Single step chemistry

Three step chemistry
1D Results
Optimal selection of the chemical parameters

<table>
<thead>
<tr>
<th></th>
<th>( \gamma ) ((0 - \nuN - \text{CJ}))</th>
<th>(Q) [MJ/kg]</th>
<th>(k ; k_C) [s(^{-1})]</th>
<th>(D_{\text{CJ}}) [m/s]</th>
<th>(T_{\nuN}) [K]</th>
<th>(l_{\text{ind}}) [(\mu\text{m})]</th>
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<tbody>
<tr>
<td>Mevel et al.</td>
<td>1.4 - 1.35 - 1.218</td>
<td>-</td>
<td>-</td>
<td>2839.9</td>
<td>1768.7</td>
<td>41</td>
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<tr>
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<td>1.33</td>
<td>4.8</td>
<td>(6 \times 10^9)</td>
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<td>1674.8</td>
<td>87.9</td>
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<td>New 1-step</td>
<td>1.35</td>
<td>4,606</td>
<td>(1.08 \times 10^{10})</td>
<td>2836.9</td>
<td>1769.5</td>
<td>36.2</td>
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<tr>
<td>Ref. 3-step</td>
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<td>4.99</td>
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<td>2850.4</td>
<td>1723.7</td>
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<tr>
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<td>(4 \times 10^7)</td>
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<td>21.4</td>
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1D Results
Chemistry: 1D fitting with critical curvature - D-kappa curves

Induction time vs. 1000/T

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- Chapman-Jouguet conditions still do not match
- Thermicity profiles are closer to the detailed chemistry result
2D Results
Numerical soot foils cell size (single-step)
2D Results
Numerical soot foils cell size (single-step)
2D Results
Numerical soot foils cell size (three-step)
2D Results

Numerical soot foils cell size (three-step)
2D Results
Interaction with an inert layer - previous results

Ref. 1-step
Ref. 3-step
Detailed

Exp. Envelopes

\( |\nabla \rho| / |\nabla \rho|_{\text{max}} \)

0.02
0.01
0.00

| \begin{tabular}{|c|}
\hline
Experimental \hline
Mevel et al. \hline
Ref. 1-step \hline
New 1-step \hline
Ref. 3-step \hline
New 3-step \hline
\end{tabular} |
<table>
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<tr>
<td>24</td>
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<tr>
<td>20</td>
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\( h_{\text{crit}} \) [mm]

2D Results

Interaction with an inert layer - promising improvement on quenching prediction (three-step)

\[
\rho / \rho_0
\]

\[
T/T_0
\]

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</tr>
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<td>New 3-step</td>
<td>&lt; 10</td>
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</table>
2D Results
Interaction with an inert layer - promising improvement on quenching prediction (three-step)

Propagated for almost 5 cm interacting with an inert gas through a 10-mm height layer

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Conclusions and future efforts

- We propose a new fitting procedure for simplified chemical kinetics

- $\kappa_{\text{crit}}$ as fitting target ($D - \kappa$ curves)

- Promising preliminary results in 2D
  - Cell size histogram better agreement with the detailed scheme
  - Critical height reduction with three-step

$$h_{\text{crit}} = 20 \text{ mm} \rightarrow h_{\text{crit}} < 10 \text{ mm}$$
Conclusions and future efforts

- We propose a new fitting procedure for simplified chemical kinetics
- $\kappa_{crit}$ as fitting target ($D - \kappa$ curves)
- Promising preliminary results in 2D
  - Cell size histogram better agreement with the detailed scheme
  - Critical height reduction with three-step
    \[ h_{crit} = 20 \text{ mm} \rightarrow h_{crit} < 10 \text{ mm} \]
- Finish the 2D analysis for quenching limits
- Variable thermodynamics
- Check our procedure for different fuels
- Extend for friction and heat losses, problem dependent
Thank you for your attention!
2D Results

Interaction with an inert layer - improve on quenching prediction (three-step)

$h = 20 \text{ mm}$

Old 3-step

Detailed

$h = 24 \text{ mm}$

$h = h_{\text{crit, 3-step}} = 20 \text{ mm}$