A new single-step reaction mechanism for propane explosions covering the entire spectrum of flame acceleration, transition to detonation and detonation

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Outline

• The new single-step reaction mechanism
• Governing equations & CFD code
• Validation
  – Comparison with detailed chemistry model
  – Detonation cell size
  – Flame acceleration in a vented duct
• Exploratory study - shock and detonation propagation through a U-bend
• Concluding remarks
Limitations of existing reaction mechanisms

(1) Berkeley GRI-mechanism (53 species, 325 reactions)
   computationally intensive

(2) Westbrook’s mechanism (1981)
   \[- \frac{d[C_3H_8]}{dt} = 8.6 \times 10^{11} \exp\left(-\frac{15000}{T}\right) [C_3H_8]^{0.1} [O_2]^{1.65}\]
   under-predicting half reaction length

(3) Frolov’s model (2007)
   \[- \frac{d[C_3H_8]}{dt} = 7 \times 10^{14} \times p^n \times \exp\left(-\frac{454600}{RT}\right) [C_3H_8] [O_2] \]
   under-predicting half reaction length for rich gas
Our group’s previous approach in detonation modelling


Reaction progress equation:

\[
\frac{\partial \rho \alpha}{\partial t} = -\nabla (\rho \alpha V) + \rho \omega
\]  

\[
\omega = A(1 - \alpha) EXP\left(-\frac{E_a}{RT}\right)
\]
The predicted overpressure and velocity vs time

The new single-step reaction mechanism

A singe-step overall reaction for propane-air combustion

\[ C_3H_8 + 5O_2 + 18.8N_2 \rightarrow 3CO_2 + 4H_2O + 18.8N_2 \]

The reaction rate in Arrhenius form

\[ \omega = k[C_3H_8]^a[O_2]^b \]

where \( k = A\exp\left(-\frac{E_a}{RT}\right) \), \([C_3H_8]\), \([O_2]\), . a and b are the rate constant, propane and oxygen molar concentrations, propane and oxygen rate exponents respectively. A and \( E_a \) denote pre-exponential factor and activation energy, respectively.
The new single-step reaction mechanism

$$\omega = k [C_3H_8]^a [O_2]^b$$

Reaction order = $a + b$

$$n = -\frac{\rho}{\tau_i} \left( \frac{\partial \tau_i}{\partial \rho} \right)_{T_0} + 1$$

The new single-step reaction mechanism

\[- \frac{d[C_3H_8]}{dt} = 3.11 \times 10^{14} \exp\left(\frac{-55910}{RT}\right)[C_3H_8]^{0.1}[O_2]^{1.65}\]
Governing equations

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \]

\[ \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right] \]

\[ \frac{\partial \rho h_s}{\partial t} + \frac{\partial \rho u_j h_s}{\partial x_j} = \frac{dp}{dt} + \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial h_s}{\partial x_j} \right) + Q \]

\[ \frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_j Y_k}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial Y_k}{\partial x_j} \right) + \omega_k \]
Numerical setup

Time: second-order Crank-Nicholson scheme

The convective terms: 2nd MUSCL scheme (TVD)

The viscous terms: second-order central differencing discretization
Validation – detonation cell size

Experimental cell width: 55mm
Predicted value: 60mm

Westbrook’s model (cell size: ~20mm)
Validation - Flame acceleration in a vented duct

Exploratory study - shock and detonation propagation through a U-bend


Width=10mm
$P_0=(60-200)\text{atm}$
$T_0=2500\text{K}$

stoichiometric propane-air mixture
$P_0=1\text{atm}$
$T_0=300\text{K}$
Numerical setup

- The geometry and set up mimics that of Frolov et al.’s experiments.
- The grid size is 0.25mm (8 grids in half reaction length) total grid number is 2.15M (10562×204)
- Six cases as listed below

<table>
<thead>
<tr>
<th>Cases</th>
<th>Initial Pressure</th>
<th>Initial Tempreature</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>150 atm</td>
<td>2500K</td>
</tr>
<tr>
<td>2</td>
<td>100 atm</td>
<td>2500K</td>
</tr>
<tr>
<td>3</td>
<td>85 atm</td>
<td>2500K</td>
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<tr>
<td>5</td>
<td>65 atm</td>
<td>2500K</td>
</tr>
<tr>
<td>6</td>
<td>60 atm</td>
<td>2500K</td>
</tr>
</tbody>
</table>
Results

The effects of the U-Bend:
(1) First decelerating and then accelerating (Cases 1 and 2)
(2) First accelerating and then decelerating (Case 3)
(3) Continuously decelerating (Case 4)
(4) Decelerating shock wave followed separately by a flame (Cases 5 and 6)
Case-1: First decelerating and then accelerating
Case 1: First decelerating and then accelerating

[Diagram showing shock wave speed and pressure variations over distance and time with labeled points PT1 to PT7 and a U-bend structure]
Case 2: First decelerating and then accelerating
Case 3: First accelerating and then decelerating
Case 4: Decelerating
Case 5: Decelerating shock wave followed separately by a flame
Case 6: Decelerating shock wave followed separately by a flame
Conclusions

• A new single-step reaction mechanism has been developed for propane-air mixture, covering the entire spectrum covering flame acceleration, transition to detonation and detonation.

• For the vented duct case, the predicted flame front is in good agreement with the measurements.

• For the six cases in the U-tube, the effects of the bend depend on the initial pressure. For the pressure range considered from 60 to 140 bar, four modes are predicted:
  - First decelerating and then accelerating
  - First accelerating and then decelerating
  - Continuously decelerating
  - Decelerating shock wave followed separately by a flame
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