3D Engine knock prediction and evaluation based on detonation theory

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Outline

I. Objective

II. Combustion model

III. Detonation theory

IV. SI Engine Application

V. Summary and Conclusions
Objective

- SI engine development tends towards downsizing and increase in compression ratio to improve efficiency
  - Increased knock tendency

- Demand on SI engine simulations
  - Predict auto-ignition events
  - Reproduce physical sensitivities
  - Predict auto-ignition as function of fuel octane ratings
  - Evaluate the transition of harmless deflagration to undesirable knocking combustion
  - Classify the severity of the auto-ignition event

Our approach:
Detailed chemistry, laminar flame speed tabulation, evaluation with the detonation diagram by Bradley
COMBUSTION MODELING
Combustion Model Approach

\[\bar{\rho} \frac{\partial \hat{G}}{\partial t} + \bar{\rho} (\hat{\mathbf{v}} \cdot \nabla) \hat{G} = \bar{\rho} s_t |\nabla \hat{G}| - \bar{\rho} D_t \tilde{k} |\nabla \hat{G}|\]

**Flame front**
- \(G = 0\)
- Chemical equilibrium

**Burnt zone**
- \(G > 0\)
- SAGE model for emission prediction

**Unburnt zone**
- \(G < 0\)
- SAGE model for auto-ignition prediction

\[s_t = s_l + u' \left\{ - \frac{c_1 c_2^2}{2c_3} Da + \left[ \left( \frac{c_1 c_2^2}{2c_3} Da \right)^2 + C_1 C_2^2 Da \right]^{1/2} \right\}\]

Laminar flame speed \(s_l\) table (via user coding)

**Figure 1:** Schematic illustration of the combustion modelling approach
Gasoline Surrogate Chemistry

- Detailed reaction mechanism
  - Latest LOGE GASOLINE
    - Fuel species (ETRF):
      - Ethanol $C_2H_5OH$
      - Toluene $A_1CH_3$
      - Iso-octane $i-C_8H_{18}$
      - N-heptane $n-C_7H_{16}$
    - Oxidation chemistry for $C_1$-$C_5$ species
    - Major exhaust-out emissions
    - Thermal NO$_x$
    - Growth pathways for poly-aromatic hydrocarbons
    - 386 species and 4511 reactions
Gasoline Surrogate Chemistry

- Skeletal scheme for auto-ignition and emissions

Detailed reaction scheme  
386 species

Horizontal lumping

Reduction: auto-ignition and major emissions  
188 species

Reduction: laminar flame speed  
78 species

Surrogate mixture formulation

Online chemistry: auto-ignition and emission prediction

Tabulation of laminar flame speed

Figure 2: Ignition delay time for a mixture of 0.72 toluene and 0.28 n-heptane (mole fraction) at $\varphi = 0.3$, $p = 10$, 30, 50 bar. Experimental data from Herzler et al. [5]

Figure 3: Ignition delay time of iso-octane/n-heptane mixtures at 40 bar, $\varphi = 1$. Experimental data from Fieweger et al. [6]
Gasoline Surrogate Chemistry

- Skeletal scheme for laminar flame speed only

<table>
<thead>
<tr>
<th>Detailed reaction scheme</th>
<th>386 species</th>
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<td>Horizontal lumping</td>
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<td>Reduction: auto-ignition</td>
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<td>laminar flame speed</td>
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Figure 4: Laminar flame speeds at 1 atm and 358 K with air as oxidizer for a mixture of 11.65% n-heptane, 36.47% iso-octane, 36.89% toluene and 15.0% ethanol (liquid volume fraction) Experimental data from Dirrenberger et al. [7]

Figure 5: Laminar flame speeds at 1 atm and 358 K with air as oxidizer for a mixture of 33.3% n-heptane, 33.33% iso-octane, and 33.3% ethanol (liquid volume fraction) Experimental data from van Lipzig et al. [8]
Gasoline Surrogate Chemistry

- **Surrogate mixture formulation**

  - Based on published correlations (Anderson et al. [3] and Morgan et al. [4])
  - Input parameters from fuel data sheet:
    - RON
    - Aromatic content (Toluene)
    - Ethanol content
  - Output: Surrogate mixture formulation

![Figure 6: Predicted MON vs. measured MON. Dashed line shows an uncertainty of 1 octane point](image)
Gasoline Surrogate Chemistry

- Tabulation of laminar flame speed
  - Table generated with LOGEsoft based on reaction scheme or correlations (faster)
  - Fast tabulation due to reduced reaction scheme
  - Tabulated in wide engine relevant range

<table>
<thead>
<tr>
<th>Property</th>
<th>Range</th>
<th>Step size</th>
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</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>1 bar to 150 bar</td>
<td>Up to 10 bar: 1 bar</td>
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<td></td>
<td>10 to 150 bar: 10 bar</td>
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<td>Unburnt zone temperature</td>
<td>350 K to 1600 K</td>
<td>50 K</td>
</tr>
<tr>
<td>Fuel-air equivalence ratio</td>
<td>0.5 to 1.5</td>
<td>0.05</td>
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<tr>
<td>EGR level</td>
<td>0 % to 30 %</td>
<td>10 %</td>
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DETONATION THEORY
Engine Knock Evaluation

- Detonation diagram by Bradley et al.

- Severity of auto-ignition event based on two dimensionless parameters:

\[ \zeta = \frac{a}{u} = a \cdot \frac{\partial T}{\partial x} \cdot \frac{\partial \tau}{\partial T} \]

\[ \varepsilon = \frac{l}{a \cdot \tau_e} \]

- speed of sound \( a \)
- reaction front velocity \( u \)
- Ignition delay time \( \tau \)
- kernel size \( l \) in which the temperature gradient is
- Excitation time \( \tau_e \) (time from 5% to maximum heat release)

**Figure 7:** Detonation diagram; Black symbols and lines: experiments Bradley et al. [1]; Grey symbols 1D simulations – open symbols: no detonation, filled symbols: developing detonation Peters et al. [9]; Colored symbols LES engine simulations: green stars: subsonic auto-ignition, blue squares: no knock, red circle: mild knock, oranges crosses: super-knock Bates et al. [10]
SI ENGINE APPLICATION
Only the most severe auto-ignition event per calculation is shown.

Transition from acceptable subsonic auto-ignition over light knock to heavy knock go well together with the predicted pressure gradients.
### Detailed Investigations

- **Investigation: severity of different ignition kernels**

CA 2.5  
CA 4.0  
CA 4.5  
CA 5.0  

![Graphs showing pressure gradient and \( \zeta \) vs. CAD for different CA values](image)

![Graph showing \( \zeta \) vs. \( \varepsilon \) for different CA values](image)
Study: same operating point with different fuel octane ratings and corresponding laminar flame speed tables

- The severity of the auto-ignition event decreases with increased fuel RON
Investigation: first appeared ignition kernel

**Sensitivity Fuel Octane Rating**

- **RON 87.0 / MON 82.4**  
  - CA 2.5
- **RON 96.0 / MON 88.2**  
  - CA 4.0
- **RON 106.9 / MON 98.7**  
  - CA 8.0

**Auto-ignition appearance CA**

**Auto-ignition severity**

**Ignition kernel size**
Conclusions

- **Engine knock prediction based on**
  - detailed chemistry
  - tabulated laminar flame speeds
  - SAGE for auto-ignition prediction

- **Physical sensitivity to**
  - spark advancing
  - fuel quality

- The knock severities based on the detonation diagram go well together with the predicted pressure traces.

- Suggested tool chain can be used efficiently to predict knock severity of different operating conditions and fuel octane ratings.
References


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