Modeling for Control of HCCI Engines

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Outline

- What is HCCI?
- Experimental test-bed at Stanford
- Motivation for modeling and control
- Proposed model
- Conclusion
- Future work
What is HCCI?

- Homogeneous Charge Compression Ignition: combustion due to uniform auto-ignition using compression alone.
  - Main Benefit: Low post-combustion temperature → reduced NOx emissions.
  - Requires: A sufficient level of inducted gas internal energy

Approaches to increasing inducted gas internal energy:

- Pre-heating the intake
- Pre-compressing the intake
- Throttling exhaust/intake → promotes hot exhaust gas re-circulation
Another Approach: Variable Valve Actuation (VVA)

with VVA:

- Exhaust reinduction achieved using late EVC
- Load variation achieved by late IVO coupled with late EVC

Benefits:

- No pumping penalty
- More control over presence of reactant/exhaust products in cylinder at any time

Challenges:

- Currently no VVA systems on production vehicle
- R&D: ongoing by many
Experimental Testbed

- Single cylinder research engine
- Fuels:
  - Propane
  - Hydrogen
  - Gasoline
- Comp. Ratio: 13:1 (adjustable)
- Engine rpm: 1800
Challenge: Combustion Phasing

- No direct combustion initiator (like spark for SI or fuel injection for Diesel combustion)

Combustion phasing depends on:

- Concentrations of reactants and re-inducted products
- Initial temperature of reactants and products

Initial Concentrations/temperature directly controlled with VVA system
Assumptions

- Homogeneous mixture
- Uniform combustion
- Complete combustion to major products

States

- volume, $V$
- temperature, $T$
- concentrations: $[X_{C_3H_8}]$, $[X_{O_2}]$, $[X_{CO_2}]$, $[X_{N_2}]$, $[X_{H_2O}]$, $[X_{CO}]$
Modeling Approach

- Volume Rate Equations
- Valve Flow Equations
- Concentration Rate Equations
- Temperature Rate Equations
- Combustion Chemistry Modeling
  - Temperature threshold approach
  - Two-step mechanism
  - Integrated Arrhenius rate threshold approach
Volume Rate Equations

\[ V = V_c + \frac{\pi B^2}{4} (l - a - \cos \theta - \sqrt{l^2 - a^2 \sin^2 \theta}) \]

\[ \dot{V} = \frac{\pi}{4} B^2 a \dot{\theta} \sin \theta (1 + a \frac{\cos \theta}{\sqrt{(L^2 - a^2 \sin^2 \theta)}}) \]

\[ \dot{\theta} = \omega \]

where:

- \( \omega \) - the rotational speed of the crankshaft
- \( a \) - is half of the stroke length
- \( L \) - connecting rod length
- \( B \) - bore diameter
- \( V_c \) - clearance volume
Valve Flow Modeling

for un-choked flow \((p_T/p_o > [2/(\gamma + 1)]^{\gamma/(\gamma-1)})\):

\[
\dot{m} = \frac{C_D A_R p_o}{\sqrt{RT_o}} \left(\frac{p_T}{p_o}\right)^{1/\gamma} \left[\frac{2\gamma}{\gamma - 1} \left[1 - \left(\frac{p_T}{p_o}\right)^{(\gamma - 1)/\gamma}\right]\right]
\]

for choked flow \((p_T/p_o \leq [2/(\gamma + 1)]^{\gamma/(\gamma-1)})\):

\[
\dot{m} = \frac{C_D A_R p_o}{\sqrt{RT_o}} \sqrt{\gamma} \left[\frac{2}{\gamma + 1}\right]^{(\gamma + 1)/2(\gamma - 1)}
\]

where:

- \(A_R\) - effective open area for the valve
- \(p_o\) - upstream stagnation pressure
- \(T_o\) - downstream stagnation temperature
- \(p_T\) - downstream stagnation pressure
The first law of thermodynamics for an open system is:

\[ \frac{d(mu)}{dt} = Q - W + \dot{m}_1 h_1 + \dot{m}_2 h_2 - \dot{m}_3 h_3 \]

- \( u \) - internal energy
- \( Q \) - heat transfer rate
- \( W = p\dot{V} \) - piston work
- \( h \) - enthalpy of species

Using the definition of enthalpy, \( h = u + pv \), and assuming no heat transfer:

\[ \frac{d(mh)}{dt} = mpV/m + pV + \dot{m}_1 h_1 + \dot{m}_2 h_2 - \dot{m}_3 h_3 \]

Assuming ideal gas and specific heats as functions of temperature, can re-write equation as a temperature rate expression.
Concentration Rate Equations

\[
\dot{X}_i = \frac{d}{dt} \left( \frac{N_i}{V} \right) = \frac{\dot{N}_i}{V} - \frac{\dot{V} N_i}{V^2} = w_i - \frac{\dot{V} N_i}{V^2}
\]

where:

- \( w_{rxn,i} \) - combustion reaction rate for species \( i \)
- \( w_{valves,i} \) - volumetric flow rate of species \( i \) through the valves
- \( N_i \) - number of moles of species \( i \) in the cylinder

\[
w_{valves,i} = w_{1,i} + w_{2,i} + w_{3,i} = (Y_{1,i} \dot{m}_1 + Y_{2,i} \dot{m}_2 - Y_{3,i} \dot{m}_3)/(V MW_i)
\]

where:

- \( Y_{1,i} \) - mass fraction of species \( i \) in the intake (constant)
- \( Y_{2,i} \) - mass fraction of species \( i \) in the exhaust (constant)
- \( Y_{3,i} = \frac{[X_i]MW_i}{\sum [X_i]MW_i} \) - mass fraction of species \( i \) in the cylinder
The rate of reaction of propane is approximated as a function of crank angle and volume following the crossing of a temperature threshold:

$$w_{C_3H_8} = \begin{cases} 
\frac{[C_3H_8]_i V_i \dot{\theta} \exp \left[ \frac{-((\theta-\theta_{init})-\bar{\theta})}{2\sigma^2} \right]}{V \sigma \sqrt{2\pi}} & T \geq T_{th} \\
0 & T < T_{th} \end{cases}$$

where:

- $\theta_{init}$ - crank angle when $T = T_{th}$
- $V_i$ - crank angle when $T = T_{th}$
- $[C_3H_8]_i$ - propane concentration when $T = T_{th}$
- $\sigma$ - crank angle standard deviation
- $\bar{\theta}$ - mean crank angle
The complete combustion of a stoichiometric propane/air mixture to major products is assumed, such that the global reaction equations is:

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

By inspection of the global reaction equation:

$$w_{O_2} = 3.5w_{C_3H_8}$$
$$w_{N_2} = 0$$
$$w_{CO_2} = -3w_{C_3H_8}$$
$$w_{H_2O} = -4w_{C_3H_8}$$
Combustion Chemistry Modeling: Temperature Threshold Approach (cont. 2)

Model Results:

IVO @ 25deg., EVC @ 165
IVO @ 45deg., EVC @ 185

Combustion phasing not captured

REASON: Combustion phasing depends on temperature AND concentrations
The rates of reaction of propane and carbon-monoxide are approximated using the following Arrhenius rate expressions:

\[
wc_3H_8 = A_1 \exp \left( \frac{-E_{A_1}}{T} \right) [C_3H_8]^m [O_2]^n
\]
\[
w_{CO,ox} = A_2 \exp \left( \frac{-E_{A_2}}{T} \right) [CO][H_2O]^o [O_2]^p
\]
\[-A_3 \exp \left( \frac{-E_{A_3}}{T} \right) [CO_2]\]

where:

- \( A \) - Pre-exponential factor
- \( E_a \) - Activation energy
The complete combustion of a stoichiometric propane/air mixture to major products is assumed through two global reactions:

\[
C_3H_8 + 3.5O_2 + 18.8N_2 \rightarrow 3CO + 4H_2O + 18.8N_2
\]

\[
CO + .5O_2 \leftrightarrow CO_2
\]

By inspection of the global reaction equations:

\[
\begin{align*}
O_2 &= 3.5C_3H_8 + .5CO_{\text{ox}} \\
N_2 &= 0 \\
CO_2 &= -CO_{\text{ox}} \\
H_2O &= -4C_3H_8 \\
CO &= -3C_3H_8 + CO_{\text{ox}}
\end{align*}
\]
Model Results:

IVO @ 25deg., EVC @ 165
IVO @ 45deg., EVC @ 185

Combustion phasing captured

Discrepancies near TDC
The rate of reaction of propane is approximated as being a function of crank angle and volume following the crossing of an integrated Arrhenius rate:

\[ w_{C_3H_8} = \begin{cases} 
\frac{[C_3H_8]_i V_i \dot{\theta} \exp \left[ -\frac{((\theta - \theta_{init}) - \bar{\theta})}{2\sigma^2} \right]}{V \sigma \sqrt{2\pi}} & \int RR \geq \int RR_{th} \\
0 & \int RR < \int RR_{th} \end{cases} \]

where:

\[ \int RR = \int_0^\theta AT^n \exp \left( \frac{E_a}{RT} \right) [C_3H_8]^a [O_2]^b d\theta \]
The complete combustion of a stoichiometric propane/air mixture to major products is assumed, such that the global reaction equations is:

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

By inspection of the global reaction equation:

\[
\begin{align*}
    w_{O_2} &= 3.5w_{C_3H_8} \\
    w_{N_2} &= 0 \\
    w_{CO_2} &= -3w_{C_3H_8} \\
    w_{H_2O} &= -4w_{C_3H_8}
\end{align*}
\]
Model Results:

- IVO @ 25deg., EVC @ 165
- IVO @ 45deg., EVC @ 185

Combustion phasing captured

Discrepancies along pressure peak
## Conclusion

### Combustion Model
- Uniform complete combustion to major products
- Three combustion chemistry models developed

### Temperature threshold approach
- Propane reaction evolves as fcn. of crank angle following temp. threshold crossing
- Does not capture combustion phasing

### Two-step mechanism
- Arrhenius rate equations implemented in two-step mechanism
- Captures combustion phasing
- Discrepancy near top dead center

### Integrated Arrhenius Rate threshold approach
- Propane reaction evolves as fcn. of crank angle following int. threshold crossing
- Captures combustion phasing
- Discrepancy along pressure peak
Future Work

- Simulate model with synthesized controller at various conditions
- Implement closed loop combustion phasing controller on research engine
- Extend model to simulate combustion phasing of more complex fuels