

1. Heat Release Modeling

Differentiate the Ideal Gas Law With Respect to Crank-Angle

$$\frac{dP}{d\theta} V + P \frac{dV}{d\theta} = mR \frac{dT}{d\theta}$$

Rearrange To Find Instantaneous Change in Pressure, Numerically Integrate To Find Pressure

$$\frac{dP}{d\theta} = \left(-\frac{P}{V} \right) \left(\frac{dV}{d\theta} \right) + \left(\frac{P}{T} \right) \left(\frac{dT}{d\theta} \right)$$

$$P(i) = P(i - 1) + \frac{dP(i)}{d\theta}$$

First Law Of Thermodynamics

$$\frac{dU}{d\theta} = \frac{dQ}{d\theta} - \frac{dW}{d\theta} \rightarrow m_{\text{dot}} C_p \left(\frac{dT}{d\theta} \right) = \frac{dQ}{d\theta} + P \frac{dV}{d\theta}$$

Rearrange to Find Instantaneous Change In Temperature, Integrate To Find Temperature

$$\frac{dT}{d\theta} = T(\gamma - 1) \left[\left(\frac{1}{PV} \right) \left(\frac{dQ}{d\theta} \right) - \left(\frac{1}{V} \right) \left(\frac{dV}{d\theta} \right) \right]$$

$$T(i) = T(i - 1) + \frac{dT}{d\theta} (i)$$

Change In Net Heat Transfer As A Function Of Crank-Angle

$$\frac{dQ}{d\theta} = \text{LHV} \frac{dX_b}{d\theta} - \frac{dQ_w}{d\theta}$$

LHV = Lower Heating Value

2. Cylinder Volume Modeling

- The engine volume (as a function of crank angle) can be calculated using engine geometry

$$V(\theta) = V_c + \frac{\pi B^2}{4} (l + a - s)$$

$$s = a \cos(\theta) + (l^2 - a^2 \sin^2 \theta)^{\frac{1}{2}}$$

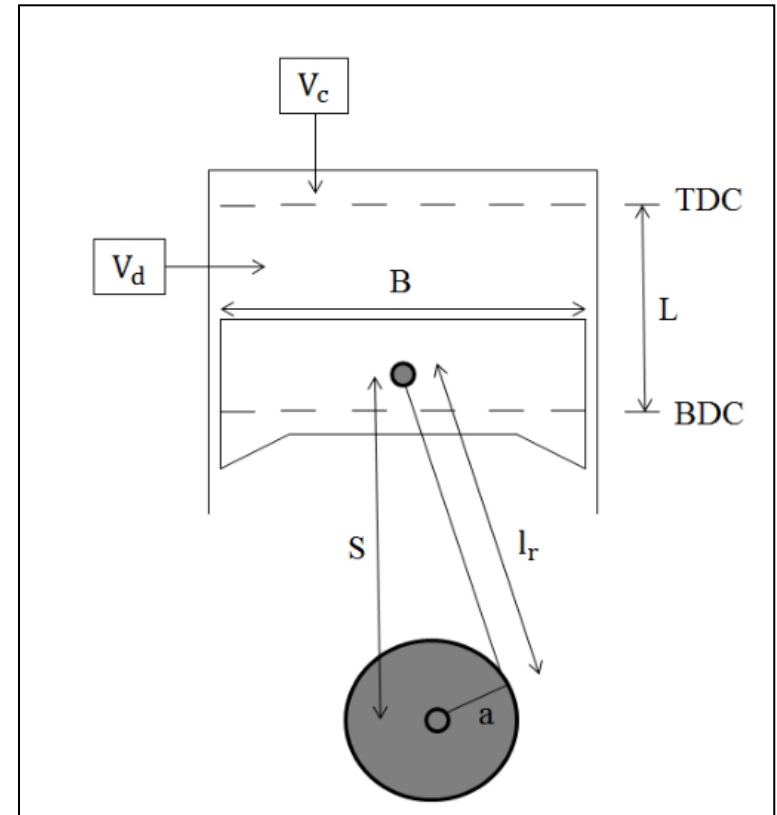
V_c =clearance volume

B =bore

l =connecting rod length

a =crank radius (1/2 of stroke)

s =instantaneous distance between piston pin and crank axis



3. Mass Fraction Burned Modeling

Weibe function is used to predict the combustion burn profile

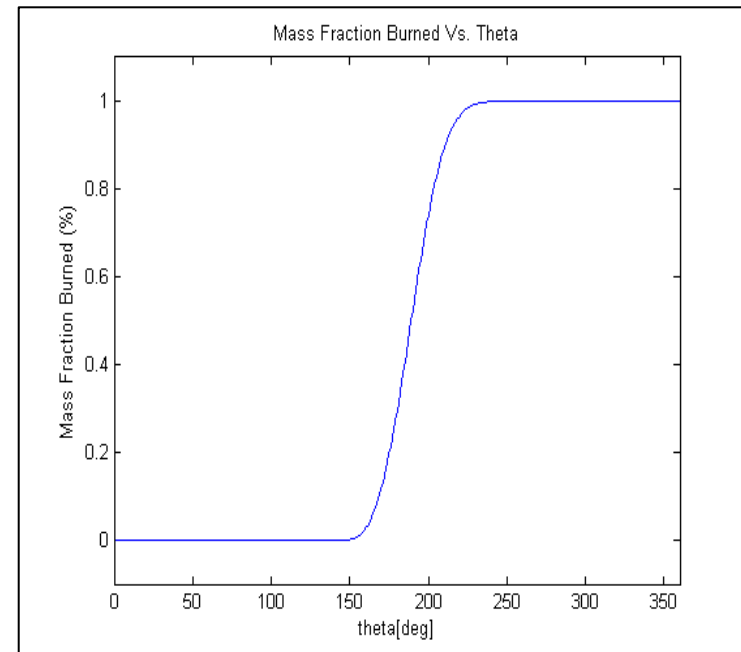
$$X_{b(\theta)} = 1 - \exp \left[-a \left(\frac{\theta(i) - \theta_o}{\theta_b} \right)^{k+1} \right]$$

$X_{b(\theta)}$ = fraction of fuel mass burned at specific crank angle

θ_o = Spark advance

θ_b = Burn duration

a, k = constants fit to a specific engine (approximately 5,2)



4. Heat Transfer Modeling

$$\frac{dQ_w}{dt} = (h_c + h_r)A_w(T - T_w)$$

h_c = convective heat transfer coefficient

h_r = radiative heat transfer coefficient

$$h_c = \frac{k_{\text{gas}} \text{Nus}}{B}$$

B = Cylinder Bore

Nus = Nusselt Number

k_{gas} = combustion gas thermal conductivity

$$k_{\text{gas}} \left(\frac{\text{W}}{\text{m} \cdot \text{K}} \right)$$
$$= 6.1944 * 10^{-3} + 7.3814 * 10^{-5}T(\text{K}) - 1.2491 * 10^{-8}T(\text{K})^2$$

$$\text{Nus} = a\text{Re}^{0.7}$$

a = 0.49 (4 – stroke engine)

$$\text{Re} = \frac{\rho_{\text{gas}} \overline{S_p} B}{\mu_{\text{gas}}}$$

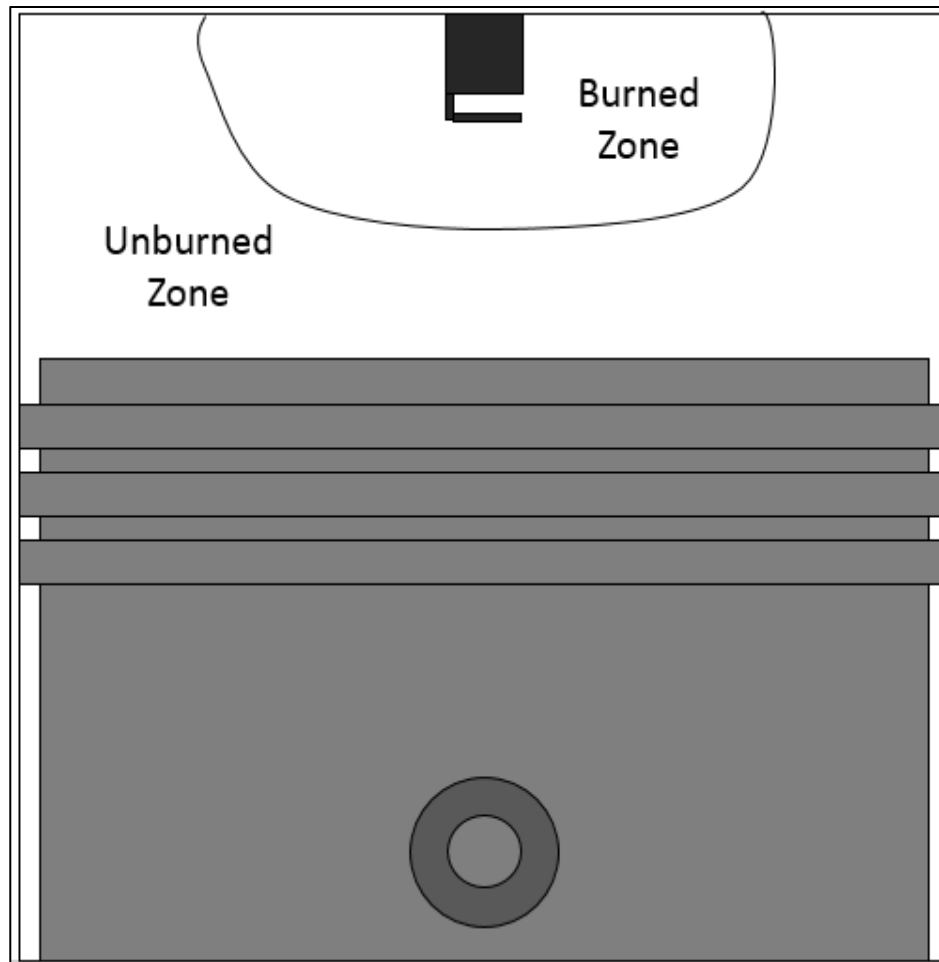
ρ_{gas} = gas density (use ideal gas law)

μ_{gas} = combustion gas viscosity

$$\mu_{\text{gas}} \left(\frac{\text{kg}}{\text{m} * \text{s}} \right) = 7.457 * 10^{-6} + 4.1547 * 10^{-8} T(\text{K}) - 7.4793 * 10^{-12} T(\text{K})^2$$

$$h_r \left(\frac{\text{W}}{\text{m}^2 * \text{K}} \right) = 4.25 * 10^{-9} \left(\frac{T^4 - T_w^4}{T - T_w} \right)$$

5. Two-Zone Model (For Burned-Zone Temperature)



$$\text{mass of air} \rightarrow m_a = \rho_a V_d$$

$$\text{mass of fuel} \rightarrow m_f = \frac{m_a}{AF_{\text{grav}}}$$

$$\text{In - cylinder mass} \rightarrow m_c = m_a + m_f$$

ρ_a = air density

AF_{grav} = gravimetric air - fuel ratio

$$\text{burned mass} \rightarrow m_b(i) = m_b(i-1) + \frac{dX_b(i)}{d\theta} m_c$$

$$\text{unburned mass} \rightarrow m_u(i) = m_u(i-1) - \frac{dX_b(i)}{d\theta} m_c$$

$$\text{unburned volume} \rightarrow V_u(i) = \left(\frac{(m_u(i)V_u(i-1))}{m_u(i-1)} \right) \left(\frac{P(i)}{P(i-1)} \right)^{\frac{1}{\gamma_u}}$$

$$\text{Total Volume} \rightarrow V(i) = V_b(i) + V_u(i)$$

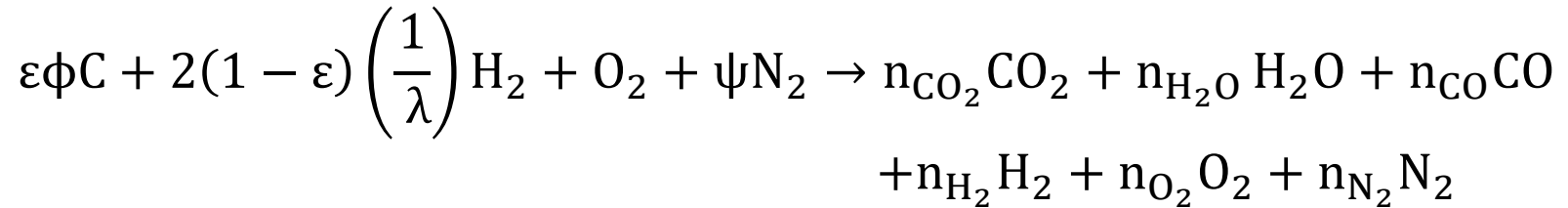
burned – zone temperature $\rightarrow T_b(i) = \frac{P(i)V_b(i)}{m_b(i)R(i)}$

unburned – zone temperature $\rightarrow T_u(i) = \frac{P(i)V_u(i)}{m_u(i)R(i)}$

$R(i)$ = instantaneous, fluid specific gas constant

This is found using the specific heat ratios model

6. Atom Balancing



$$\varepsilon = \frac{4}{4 + y}$$

n_i = molar concentration of each species per mole of O_2 reactant

Ψ = molar nitrogen – to – oxygen ratio of air (3.773)

y = molar hydrogen – to – carbon ratio of fuel

Species	$\lambda > 1$	$\lambda \leq 1$
CO ₂	$\varepsilon \left(\frac{1}{\lambda} \right)$	$\varepsilon \left(\frac{1}{\lambda} \right) - c$
H ₂ O	$2(1 - \varepsilon) \left(\frac{1}{\lambda} \right)$	$2 \left(1 - \varepsilon \left(\frac{1}{\lambda} \right) \right) + c$
CO	0	c
H ₂	0	$2 \left(\left(\frac{1}{\lambda} \right) - 1 \right) - c$
O ₂	$1 - \left(\frac{1}{\lambda} \right)$	0
N ₂	ψ	ψ
Total: n _{tot}	$(1 - \varepsilon) \left(\frac{1}{\lambda} \right) + 1 + \psi$	$(2 - \varepsilon) \left(\frac{1}{\lambda} \right) + \psi$

Water – Gas Shift Reaction \rightarrow $\text{CO}_2 + \text{H}_2 \leftrightarrow \text{CO} + \text{H}_2\text{O}$

$$K_{\text{WGS}} = \frac{n_{\text{H}_2\text{O}} n_{\text{CO}}}{n_{\text{CO}_2} n_{\text{H}_2}}$$

$$K_{\text{wgs}}(T) = \exp\left(2.743 - \frac{1.761 \times 10^3}{T_b(\text{K})} - \frac{1.611 \times 10^6}{T_b(\text{K})^2} + \frac{0.2803 \times 10^9}{T_b(\text{K})^3}\right)$$

7. NO Formation Model

zeldovich mechanism $\rightarrow \frac{d[\text{NO}]}{dt} = 2k_{1f}[\text{N}_2]_e[\text{O}]_e$

$[\text{N}_2]_e$ = equilibrium concentration of N_2

$[\text{O}]_e$ = equilibrium concentration of O

k_{1f} = forward reaction rate coefficient

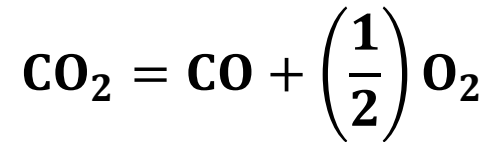
$$k_{1f} \left(\frac{\text{cm}^3}{\text{gmol} \cdot \text{s}} \right) = (1.82 * 10^{14}) \exp \left(- \frac{38370}{T_b} \right)$$

$$[O]_e = \frac{k_o [O_2]_e^{\frac{1}{2}}}{(R_u T_b)^{\frac{1}{2}}}$$

$$R_u = \text{Universal Gas Constant} \left(8315 \left[\frac{\text{J}}{\text{kmol} \cdot \text{K}} \right] \right)$$

$$K_o \left(\text{Pa}^{\frac{1}{2}} \right) = 3.6 \times 10^3 \exp \left(- \frac{31090}{T_b} \right) \times (101325)^{\frac{1}{2}}$$

The equilibrium concentration of O_2 is found using the following equilibrium equation:



The equilibrium constant can be calculated as a function of the burned zone temperature using the JANAF tables:

$$\log_{10} K_p = K_{pCO_2} - K_{pCO}$$

Use the following equation to calculate the percentage of dissociation of CO₂:

$$\frac{1 - \alpha}{\alpha \left(\frac{\alpha}{2}\right)^{\frac{1}{2}}} \left(\frac{n_p}{P_p}\right)^{\frac{1}{2}} = K_p$$

$$\frac{n_p}{P_p} = \frac{1.5}{P_{EXH}} \left(\frac{T_b}{T_{BDC}}\right)$$

Assume that the equilibrium mole fraction of nitrogen is equal to that provided by the atom balance equations. Assume that the composition is frozen at 90% of the peak burned-zone temperature.

8. Hydrocarbon Emissions Model (flame-quenching)

Unburned Gas Fraction $\rightarrow f_{\text{unburned}} = 1 - X_r - \text{EGR}$

X_r = residual gas fraction

EGR = fraction of exhaust gas recirculated

Fuel Vapor Fraction $\rightarrow f_{\text{vapor}} = \frac{1}{1 + AF_{\text{mol}}}$

AF_{mol} = molar air – fuel ratio

$$\text{Spark Plug Correction Factor} \rightarrow f_{\text{plug}} = 1 - 0.85 \left(\frac{d_{\text{splug}}(\text{m})}{B(\text{m})} \right)$$

d_{splug} = distance of spark – plug offset from piston center axis

This is total crevice emissions index. A further explanation of HC formation mechanisms can be found on the Mindworks website.

$$SF_{\text{crevice}} = 5443 \left(\frac{P_{\text{peak}}}{\text{IMEP}} \right) \left(\frac{V_{\text{crevice}}}{\frac{V_d}{N_{\text{cyl}}}} \right) \left(\frac{1}{T_{\text{coolant}}(\text{K})} \right) (f_{\text{unburned}})(f_{\text{vapor}})(f_{\text{plug}})$$

The peak cylinder pressure and IMEP can be found from the single-zone model. The coolant temperature can be estimated as 350 [K]. The crevice volume can be measured.

8. Hydrocarbon Emissions Model (Oil Layer Absorption and Desorption)

$$\text{mass of oil film} \rightarrow m_{\text{oil}} = \rho_{\text{oil}} \pi \delta_{\text{oil}} B S$$

$$\rho_{\text{oil}} = \text{oil density} \sim 900 \left[\frac{\text{kg}}{\text{m}^3} \right]$$

$$\delta_{\text{oil}} = \text{oil layer thickness} \sim 3 [\mu\text{m}]$$

$$\text{mass of HC} \rightarrow m_{\text{HC}} = P_{\text{est}} \left(\frac{1}{AF_{\text{mol}}} \right) \left(\frac{MW_{\text{air}}}{MW_{\text{HC}}} \right) \left(\frac{MW_{\text{HC}}}{MW_{\text{oil}} H} \right) m_{\text{oil}}$$

MW_i = constituent molecular weights

H = Henry's Constant

The pressure term used in predicting the mass of hydrocarbons can be estimated as an average between the inlet and peak combustion temperatures.

$$P_{\text{est}} = \left(\frac{1}{2}\right) (P_{\text{inlet}}(\text{atm}) + P_{\text{inlet}}(\text{atm})R_c^Y)$$

$$P_{\text{inlet}}(\text{atm}) = 0.09875 + 0.00986\text{IMEP}(\text{kPa})$$

$$\text{SF}_{\text{wall}} = 63024 \left(\frac{1}{\text{IMEP}(\text{kPa})}\right) \left(\frac{1}{\text{AF}_{\text{mol}}(10^{0.0082T_{\text{oil}}(\text{K})})B(\text{m})}\right) P_{\text{est}}$$