A User-Friendly, Two-Zone Heat Release and Emissions Model

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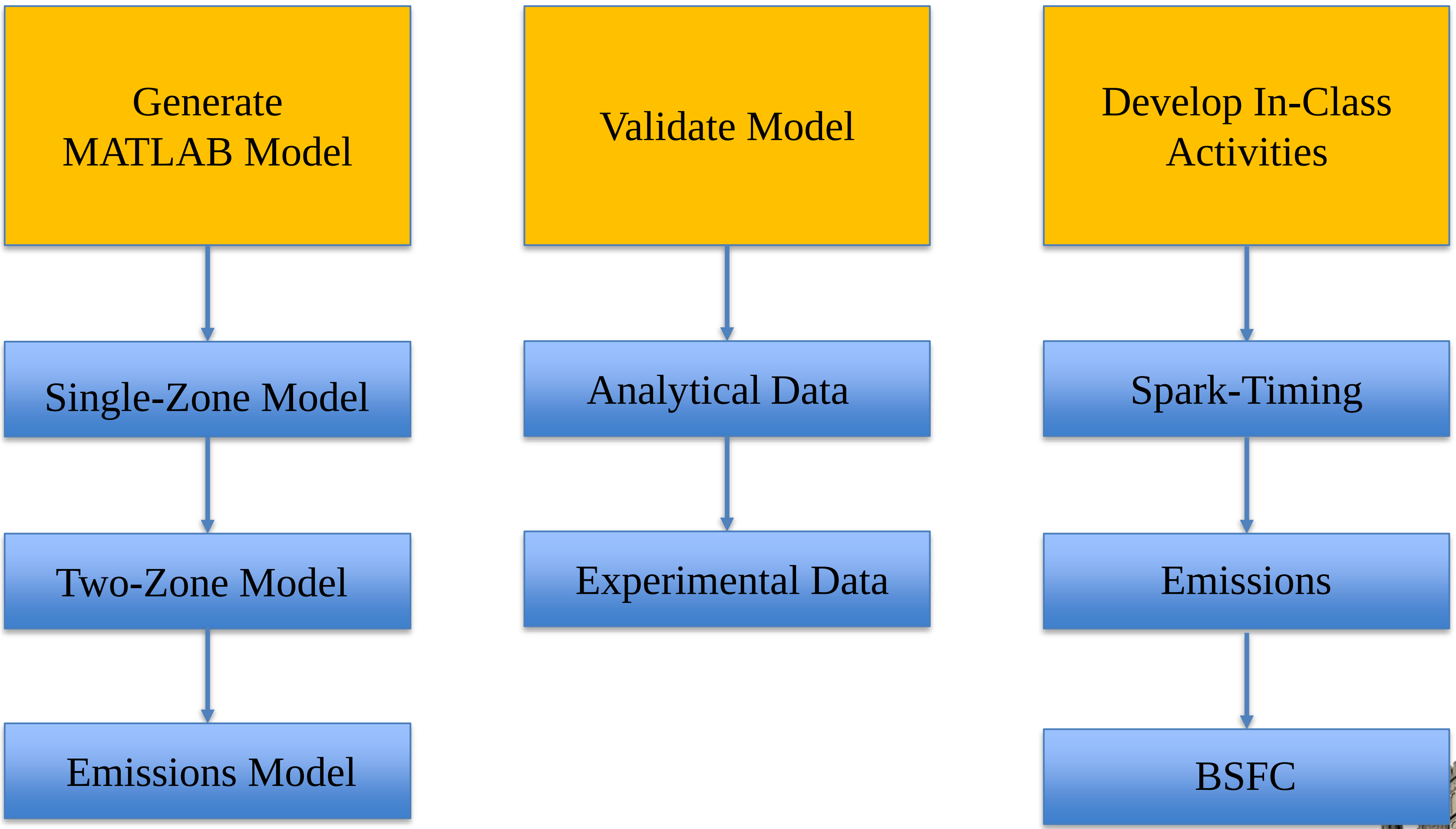
Objectives



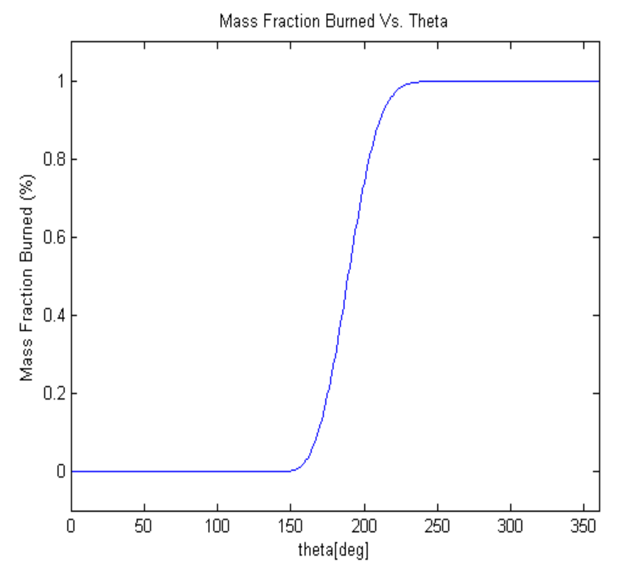
- Generate MATLAB Model
  - Single-Zone Model
  - Two-Zone Model
  - Emissions Model
- Validate Model
  - Analytical Data
  - Experimental Data
- Develop In-Class Activities
  - Spark-Timing
  - Emissions
  - BSFC

Weibe Function

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)



- Can be fit a specific engine with a measured pressure trace (using polytropic relationships)

Cylinder Volume

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

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

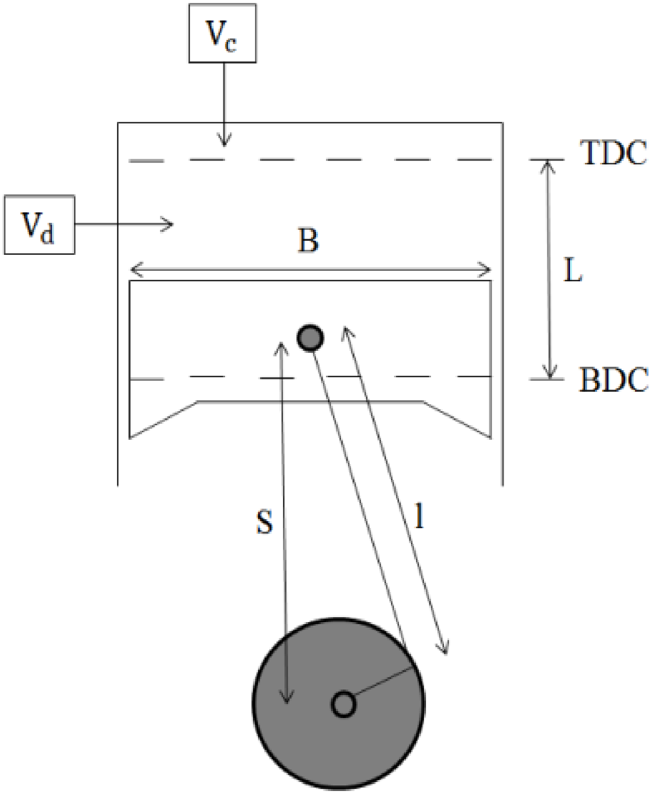
V_c=clearance volume

B=bore

l=connecting rod length

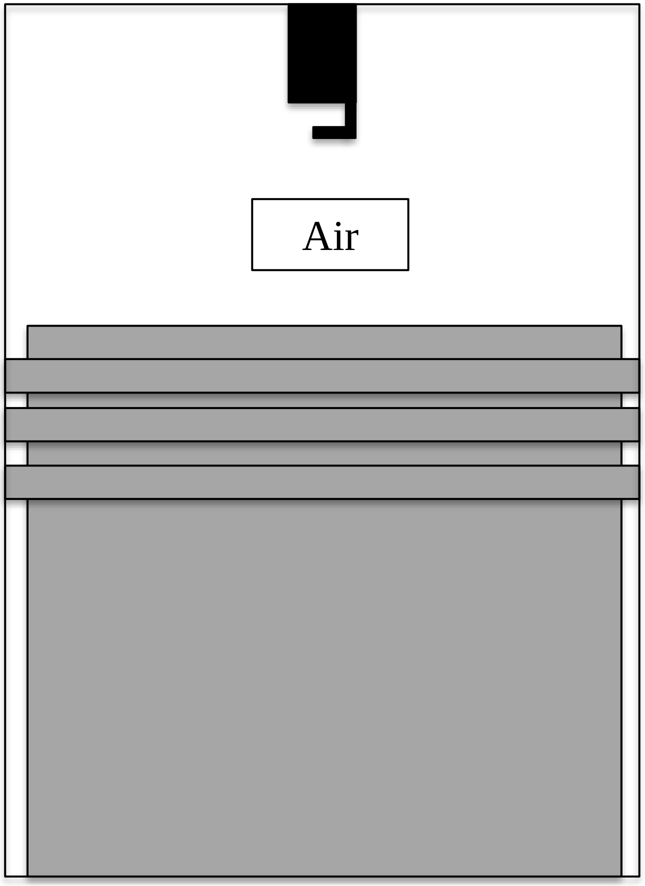
a=crank radius (1/2 of stroke)

s=instantaneous distance between piston pin and crank axis



Single-Zone Model

- Combustion chamber is treated as a single, ideal gas (air).
- Bulk temperature and pressure profiles are predicted using the ideal gas law.
- Used to predict a pressure trace, engine power.
- Bulk, average temperature is ineffective in predicting emissions.



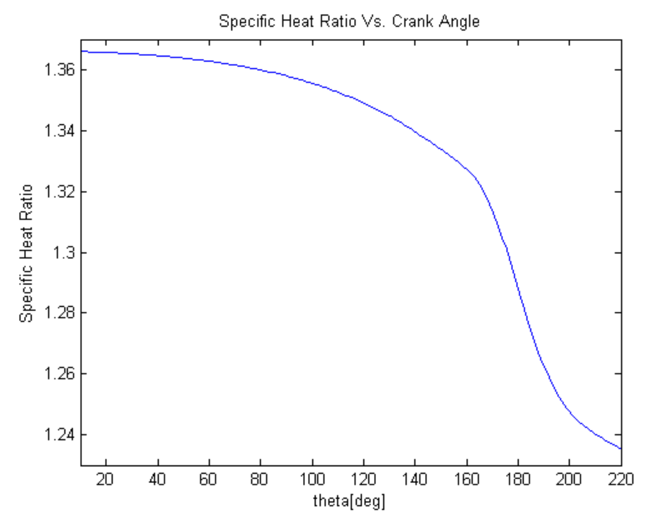
Single-Zone Modifications

- Engine friction can be modeled linearly. Empirical equations can be found for many applications (motorcycle shown)

$$\text{fmep} = 250(L)(RPM)$$

L = stroke

- The specific heat ratio can be modeled as a function of temperature. A curve-fitted equation was used in this model.



Two-Zone Model

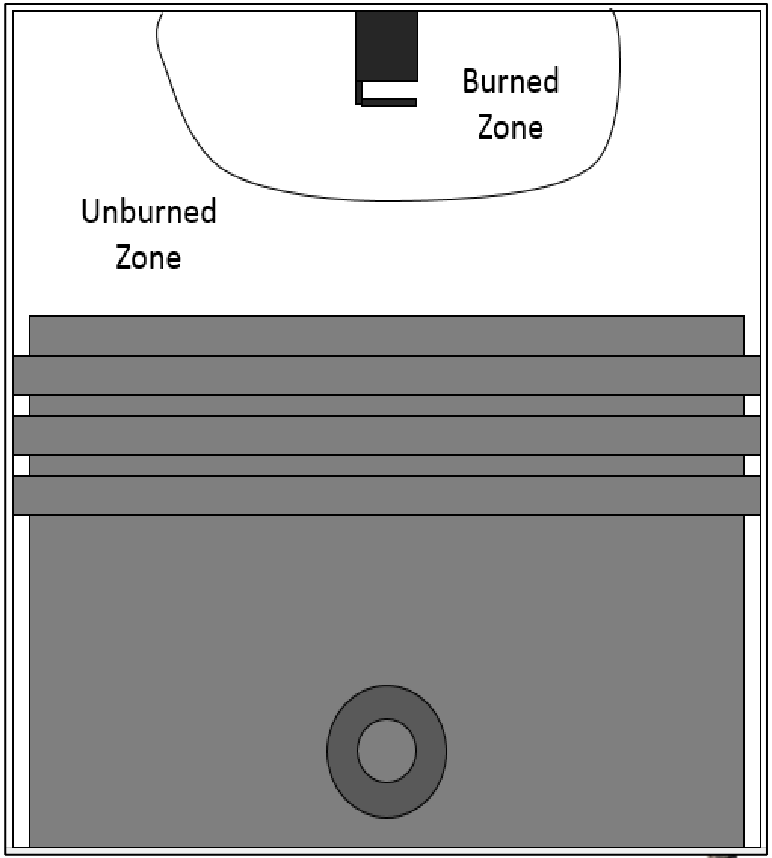
- Splits the single zone model into “burned” and “unburned” zones.

$$1.)\ m_u(i) = m_u(i-1) + \frac{dX_b}{d\theta}(i)m_c$$

$$2.)\ V_u(i) = \left(\frac{m_u(i)V_u(i-1)}{m_u(i-1)}\right)\left(\frac{P(i)}{P(i-1)}\right)^{\frac{1}{\gamma_u}}$$

$$3.)\ V(i) = V_u(i) + V_b(i)$$

- Elevated “Burned” zone temp. is used to predict emissions.
- Can’t be used for power predictions (discontinuous Temp. Profile).



Heat Transfer Prediction Methods

•Heat transfer prediction methods are derived from Newton’s law of cooling.

$$\frac{dQ_w}{dt} = hA(T - T_w)$$

T_w=wall temperature (constant)
A=instantaneous heat transfer area
h=heat transfer coefficient

•Both methods use empirical equations to calculate “h”.

- Woschni’s method splits process into respective combustion periods.
- Woschni assumed gas velocities were proportional to the mean piston speed.
- Annand included radiative terms. Annand assumed “pipe flow characteristics”.

Modeling NO Formation

Formation Mechanisms

(1) Zeldovich mechanism

High Temperature Combustion (above 1800 K)

(2) The prompt mechanism

Low Combustion Temperatures, When Fuel Contains Nitrogen

(3) The N_2O-intermediate mechanism

Lean, Low Temperature Combustion

(4) The NNH mechanism

Least Understood, Important in Hydrogen Combustion

- Only the general Zeldovich mechanism was used in this model:

$1.)\ O + N_2 \overrightarrow{k_{1_f}} NO + N$

$2.)\ N + O_2 \overrightarrow{k_{2_f}} NO + O$

Modeling NO Formation Continued

- Rate of NO formation is expressed as:

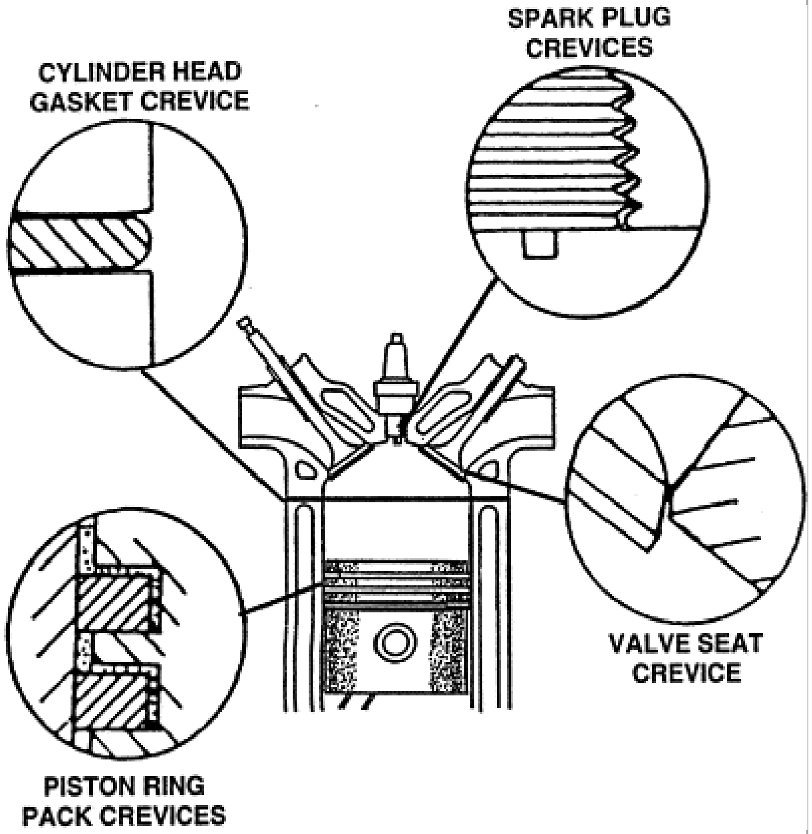
$$\frac{d[NO]}{dt} = 2k_{1f}[O]_e[N_2]_e$$

- k_{1f} (forward reaction rate coefficient) was found using an Arrhenius equation and values from a lookup-table.
- Rich combustion required equilibrium constants for the water-gas-shift reaction and dissociation of CO_2.

Water-Gas Shift Reaction	$CO_2 + H_2 \leftrightarrow CO + H_2O$
Dissociation of CO_2	$CO_2 \leftrightarrow CO + \left(\frac{1}{2}\right) O_2$

HC Emissions Due to Crevices

- Flames require a minimum distance in order to propagate through an opening, otherwise the flame is extinguished.
- In cold-engine operation, crevices and cylinder walls also work as a heat sink creating fuel pooling.
- This model included piston ring pack crevices and a correction factor due to spark-plug offsets.



HC Oil Layer Absorption and Desorption

- HC molecules absorb into the oil film on the intake and compression cycles.
- HC continue to absorb past saturation due to rising vapor pressures (reference Henry’s Law).
- The post-combustion imbalance in concentrations (between the oil layer and combustion chamber gases) causes HC desorption.

Henry’s Law →

$$x_a = \frac{p_a}{H}$$

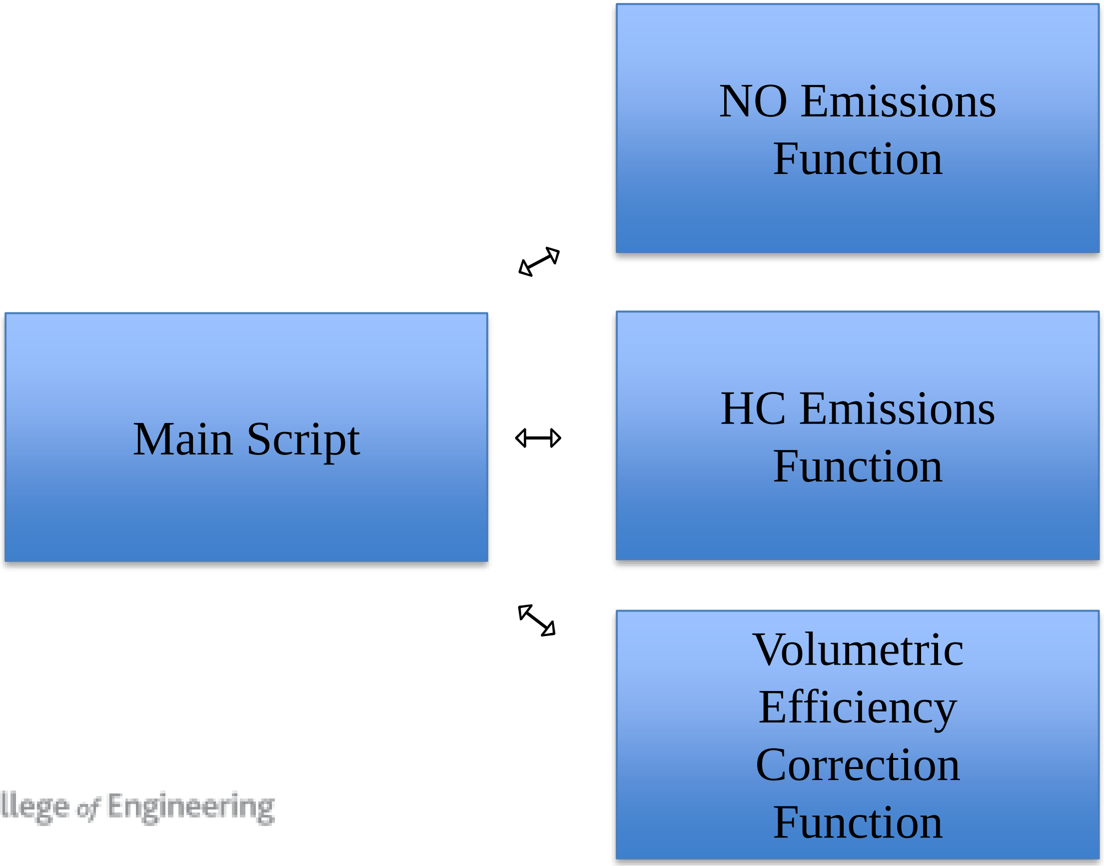
$x_a = \text{mole fraction of "a“}$

$p_a = \text{partial pressure of "a"}$

$H = \text{Henry's Constant}$

MATLAB Model

- The main MATLAB simulation was stored in a script.
- Functions were generated to predict emissions and volumetric efficiencies.
- Sub-functions were created to plot BSFC and emissions maps.



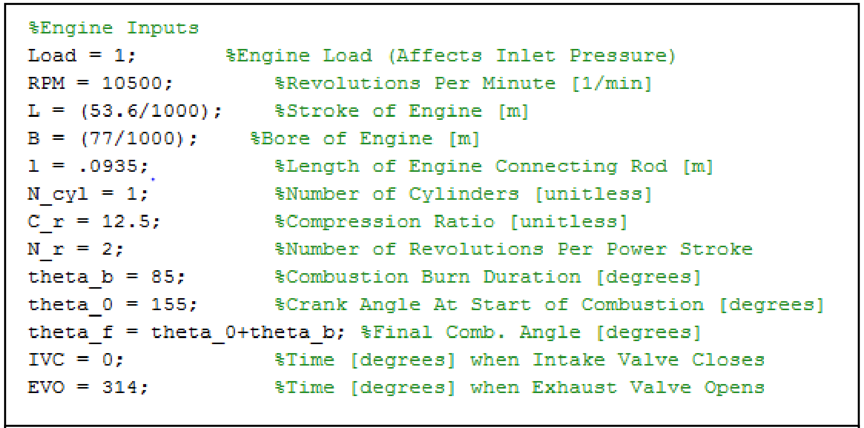
NO Emissions Function

Main Script

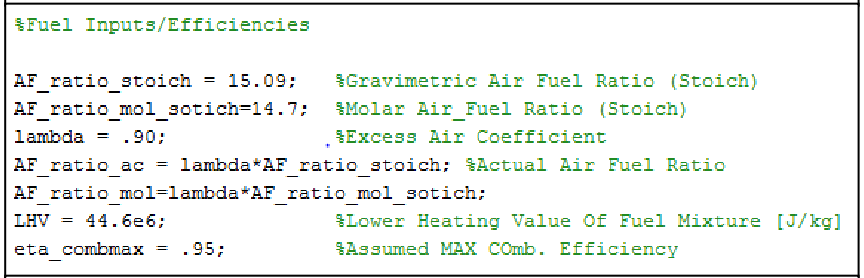
HC Emissions Function

Volumetric Efficiency Correction Function

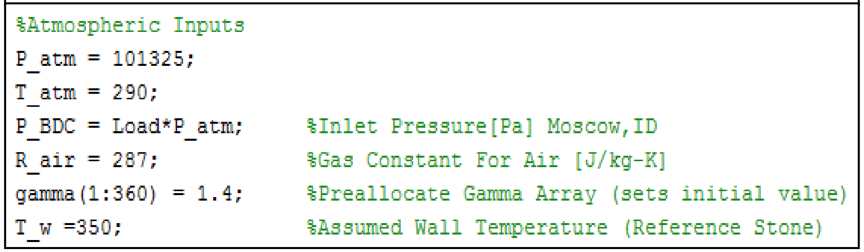
Model Inputs



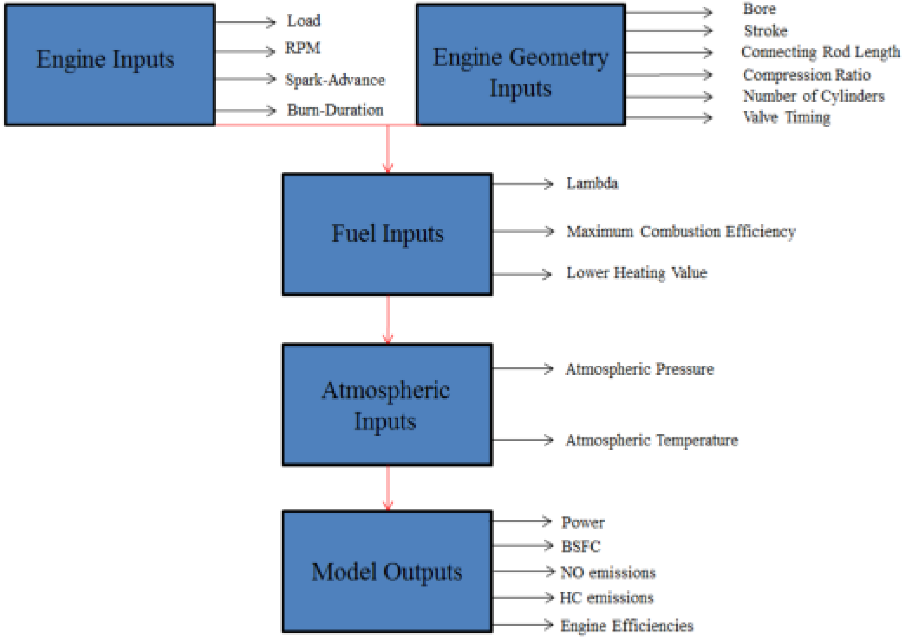
```
%Engine Inputs
Load = 1;        %Engine Load (Affects Inlet Pressure)
RPM = 10500;         %Revolutions Per Minute [1/min]
L = (53.6/1000);     %Stroke of Engine [m]
B = (77/1000);     %Bore of Engine [m]
l = .0935;           %Length of Engine Connecting Rod [m]
N_cyl = 1;           %Number of Cylinders [unitless]
C_r = 12.5;          %Compression Ratio [unitless]
N_r = 2;             %Number of Revolutions Per Power Stroke
theta_b = 85;        %Combustion Burn Duration [degrees]
theta_0 = 155;       %Crank Angle At Start of Combustion [degrees]
theta_f = theta_0+theta_b; %Final Comb. Angle [degrees]
IVC = 0;             %Time [degrees] when Intake Valve Closes
EVO = 314;           %Time [degrees] when Exhaust Valve Opens
```



```
%Fuel Inputs/Efficiencies

AF_ratio_stoich = 15.09;   %Gravimetric Air Fuel Ratio (Stoich)
AF_ratio_mol_sotich=14.7;  %Molar Air_Fuel Ratio (Stoich)
lambda = .90;              %Excess Air Coefficient
AF_ratio_ac = lambda*AF_ratio_stoich; %Actual Air Fuel Ratio
AF_ratio_mol=lambda*AF_ratio_mol_sotich;
LHV = 44.6e6;              %Lower Heating Value Of Fuel Mixture [J/kg]
eta_combmax = .95;         %Assumed MAX COmb. Efficiency
```

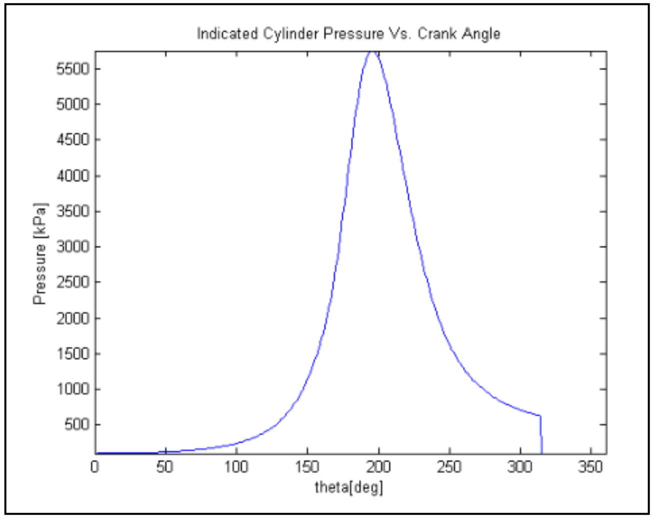


```
%Atmospheric Inputs
P_atm = 101325;
T_atm = 290;
P_BDC = Load*P_atm;     %Inlet Pressure[Pa] Moscow,ID
R_air = 287;            %Gas Constant For Air [J/kg-K]
gamma(1:360) = 1.4;     %Preallocate Gamma Array (sets initial value)
T_w =350;               %Assumed Wall Temperature (Reference Stone)
```

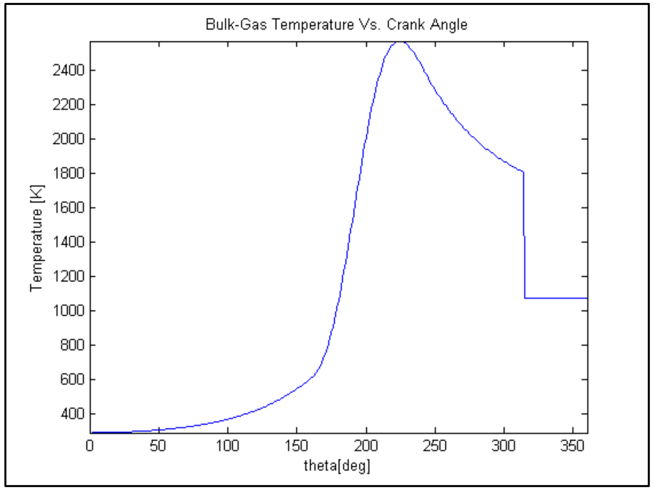


Single-Zone Outputs

- The indicated cylinder pressure is predicted using the single-zone model.
- EVO cuts the plot off.
- IVC causes pressure to begin building.

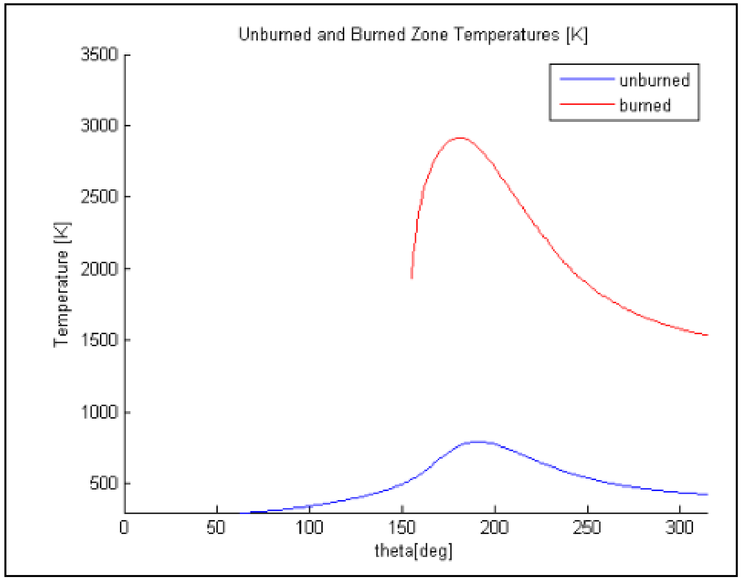


- The bulk cylinder temperature is produced using the single-zone model.
- This is the average of the burned and unburned zones.

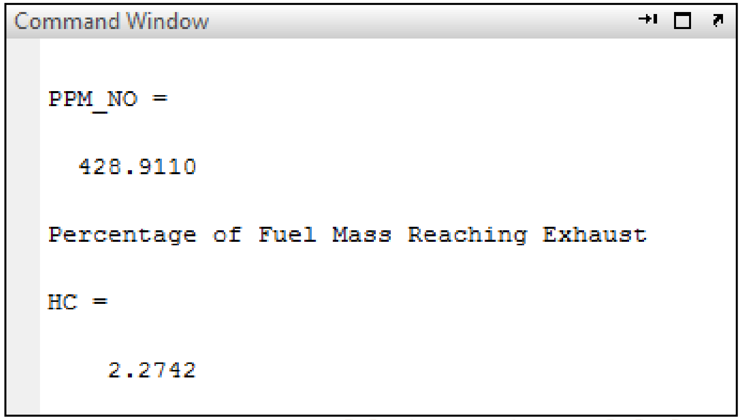


Two-Zone Outputs

- The two-zone model splits the bulk temperature into unburned and burned-zones.
- The burned-zone temperature is elevated in comparison to the bulk gas temperature.

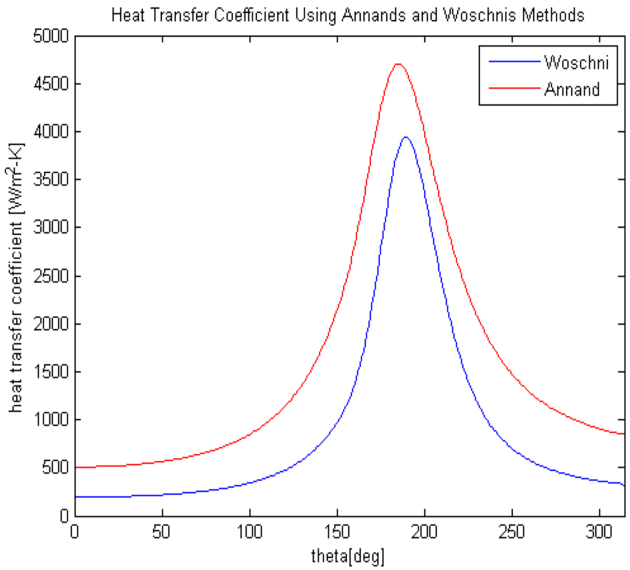


- HC and NO emissions are displayed in the command window.
- Frozen NO composition was assumed at 90% of the peak burned-zone temperature.



```
PPM_NO =

  428.9110

Percentage of Fuel Mass Reaching Exhaust

HC =

    2.2742
```

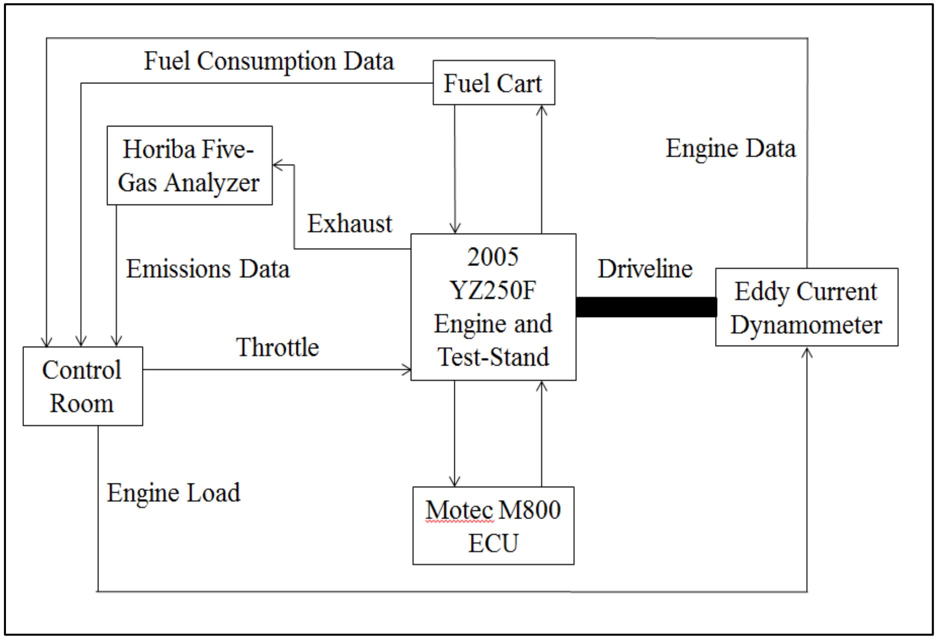
Comparing Model Outputs



Variable	**Woschni**	**Annand**	**Relative Error**
NO	429.57[PPM]	341.19[PPM]	20.57 [%]
HC	2.47 [%]	2.27 [%]	8.10[%]
Power	24.40 [kW]	22.76 [kW]	6.72[%]
BMEP	1117.20[kPa]	1042.10 [kPa]	6.72[%]
BSFC	334.30 [g/kW-h]	353.51 [g/kW-h]	5.75[%]
Mechanical Efficiency	88.81 [%]	88.81 [%]	0[%]
Combustion Efficiency	85.09 [%]	85.09 [%]	0[%]

- Woschni’s method under-predicted the heat transfer coefficient
- Woschni’s method over-predicted torque and NO emissions.
- Since NO formation is strongly temperature dependent, the 20% relative error shown was due to a difference in formation temperatures of approximately 120[K]

Experimental Setup



Fuel Consumption Data

Fuel Cart

Horiba Five-Gas Analyzer

Engine Data

Exhaust

Emissions Data

2005 YZ250F Engine and Test-Stand

Driveline

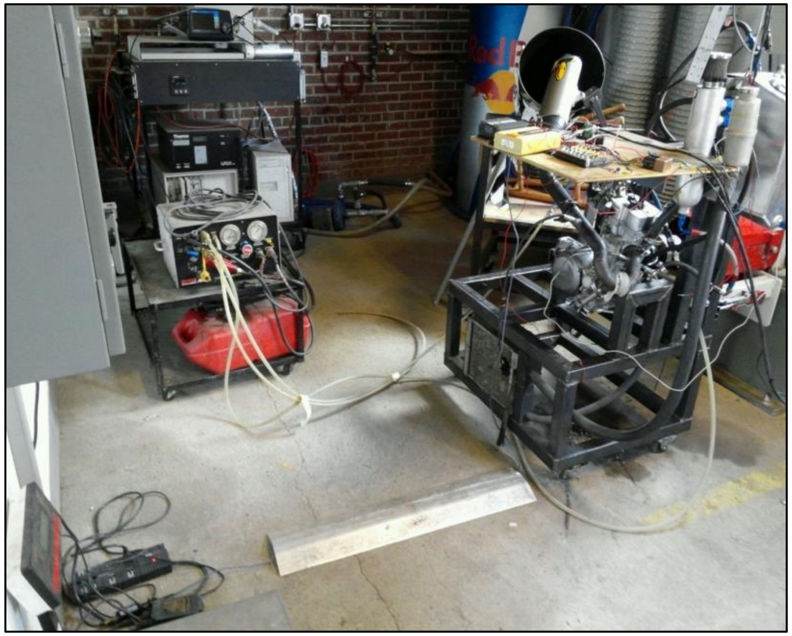
Eddy Current Dynamometer

Throttle

Control Room

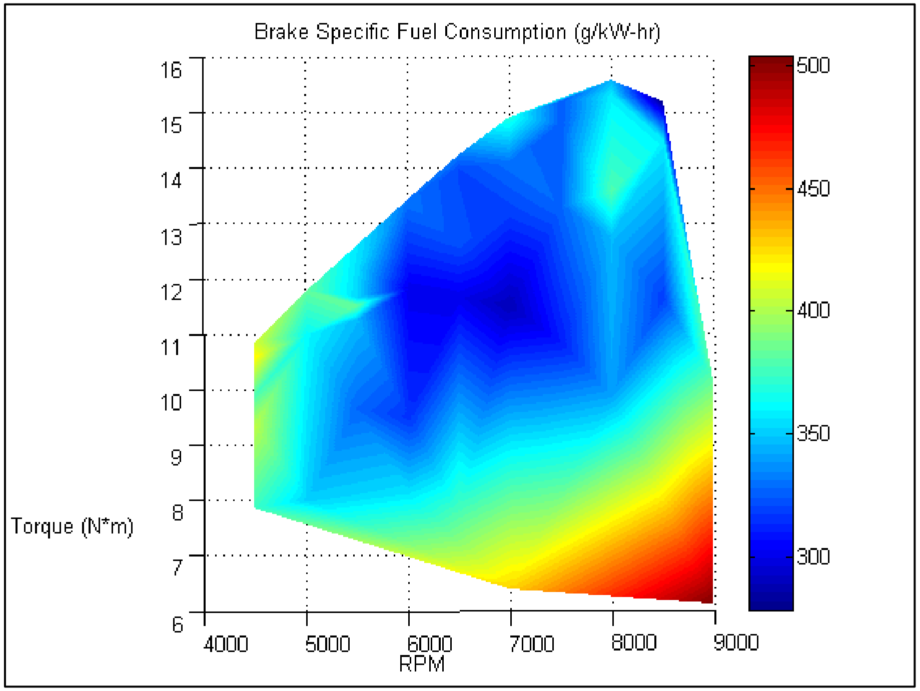
Engine Load

Motec M800 ECU



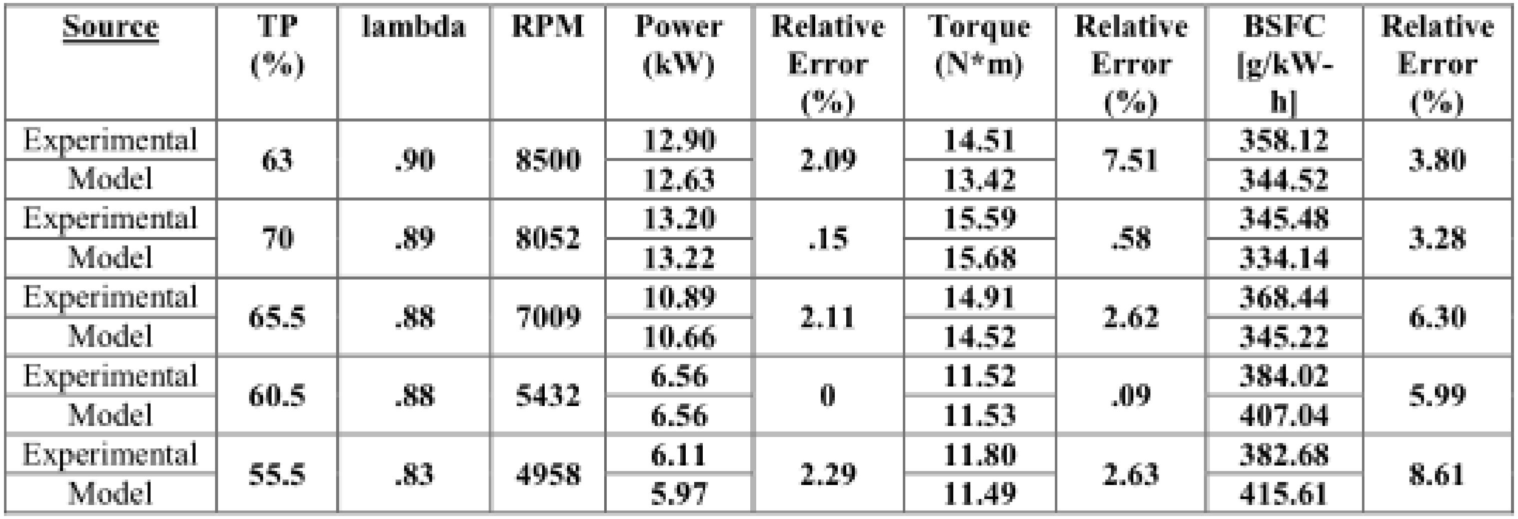
Acquired Data

- The BSFC map showed a trough in the plot at the upper right corner (~8500 RPM, 70% throttle).
- During Testing, the engine seized, so a complete map wasn't possible.
- Over testing range, minimum BSFC values were ~280[g/kW-h]



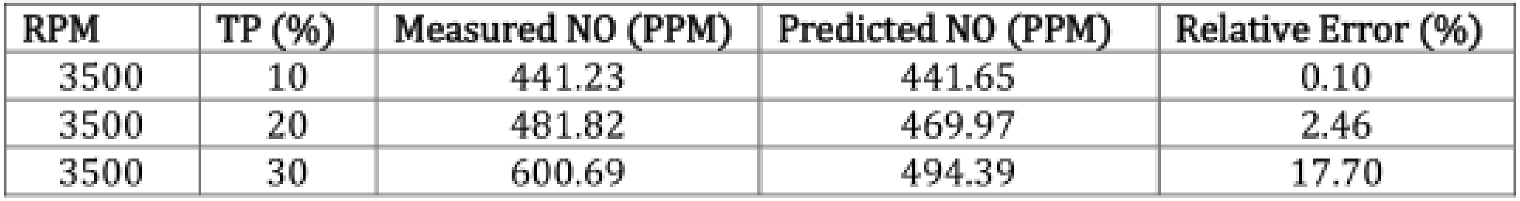
Comparing Data to Model

Power, Torque, BSFC



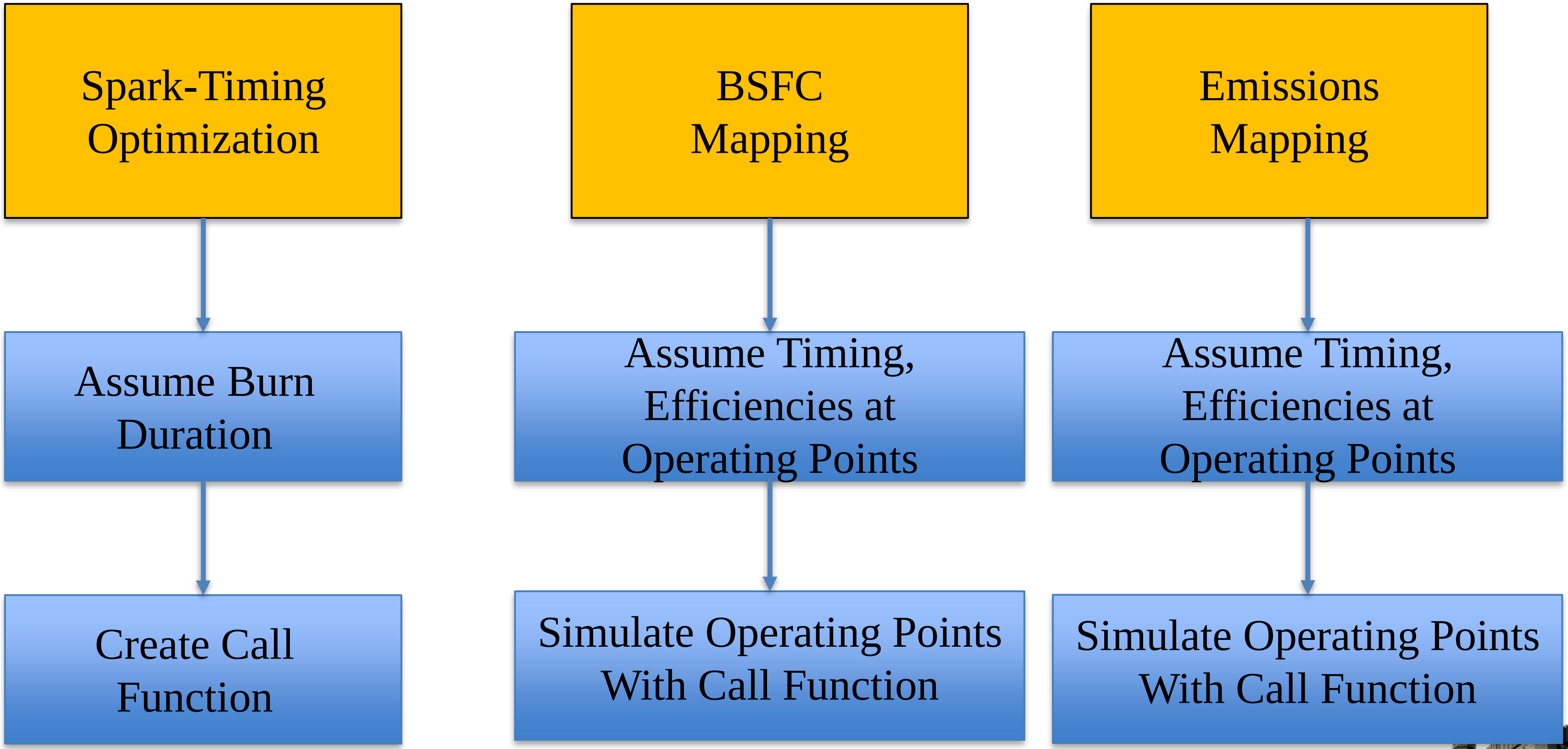
Source	TP (%)	lambda	RPM	Power (kW)	Relative Error (%)	Torque (N*m)	Relative Error (%)	BSFC [g/kW-h]	Relative Error (%)
Experimental	63	.90	8500	12.90	2.09	14.51	7.51	358.12	3.80
Model				12.63		13.42		344.52	
Experimental	70	.89	8052	13.20	.15	15.59	.58	345.48	3.28
Model				13.22		15.68		334.14	
Experimental	65.5	.88	7009	10.89	2.11	14.91	2.62	368.44	6.30
Model				10.66		14.52		345.22	
Experimental	60.5	.88	5432	6.56	0	11.52	.09	384.02	5.99
Model				6.56		11.53		407.04	
Experimental	55.5	.83	4958	6.11	2.29	11.80	2.63	382.68	8.61
Model				5.97		11.49		415.61	

NO Emissions



RPM	TP (%)	Measured NO (PPM)	Predicted NO (PPM)	Relative Error (%)
3500	10	441.23	441.65	0.10
3500	20	481.82	469.97	2.46
3500	30	600.69	494.39	17.70

In-Class Activities



Spark-Timing Optimization

Assume Burn Duration

Create Call Function

BSFC Mapping

Assume Timing, Efficiencies at Operating Points

Simulate Operating Points With Call Function

Emissions Mapping

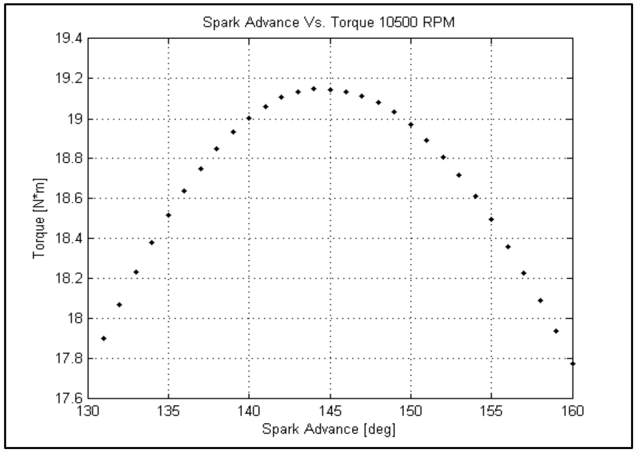
Assume Timing, Efficiencies at Operating Points

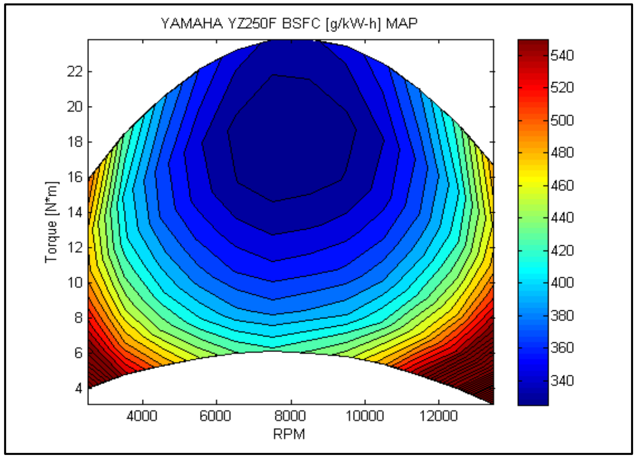
Simulate Operating Points With Call Function

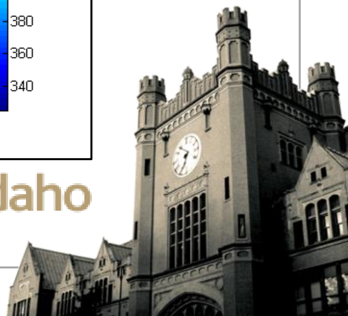
Spark-Timing and BSFC Plots

- An MBT spark-timing plot was constructed .
- This required an assumed air-fuel ratio and burn duration.

- The BSFC map required functions that simulated many loads, RPM, and assumed air-fuel ratios.
- A burn-duration model would improve the accuracy of the plot shown.
- The model also predicts throttle positions that may not be possible to operate at (i.e. 4000 RPM 100% throttle)



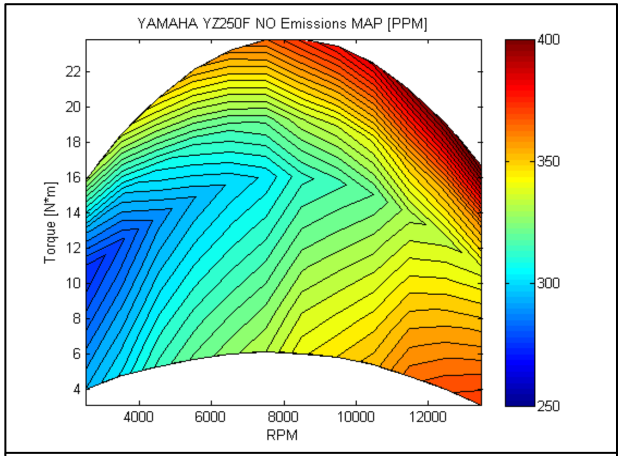


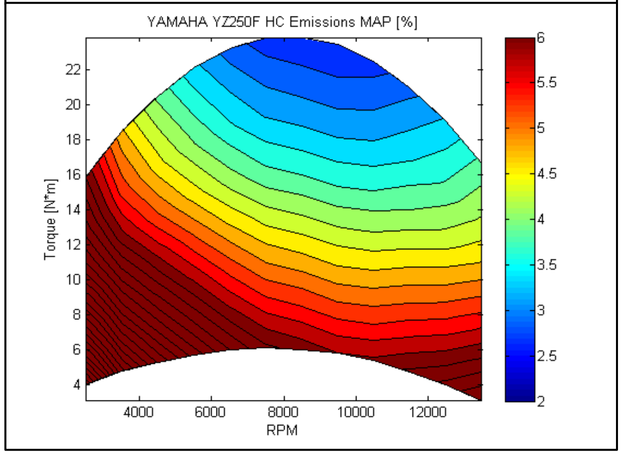


Emissions Maps

- The same functions that were used to create BSFC maps were used to create emissions maps.
- NO emissions ranged relative to combustion temperatures and air-fuel ratios.

- HC emissions were high at low loads.
- HC emissions were related to combustion temperatures and the “quality” of combustion.

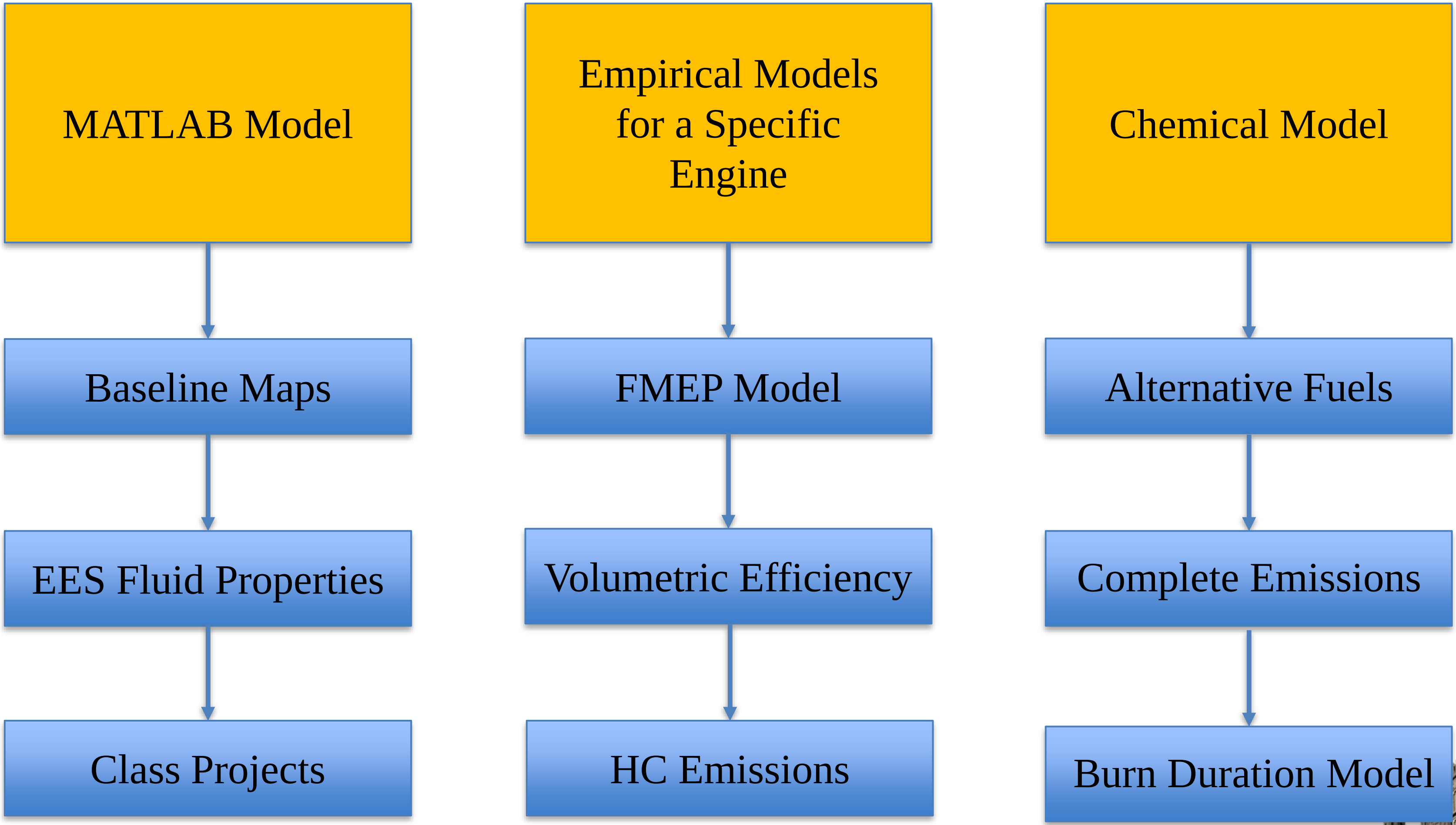




Conclusions

- The model was valid at operating points from 50%-70% throttle.
- No data points above 70% throttle and at high engine speeds were gathered due to engine failure.
- A volumetric efficiency map at low throttle positions would be necessary.
- It’s expected that relative error in BSFC calculations could be minimized by documenting fuel temperatures.

Future Work



MATLAB Model

Baseline Maps

EES Fluid Properties

Class Projects

Empirical Models for a Specific Engine

FMEP Model

Volumetric Efficiency

HC Emissions

Chemical Model

Alternative Fuels

Complete Emissions

Burn Duration Model

Questions?