EML 4930/5131: Combustion
Computer Project 2
Due Wednesday, December, 2021

Report Format

Please turn in a separate typed report (MS Word, LaTeX, etc.) with the plots embedded into the document. In addition, email your python scripts, IPython notebooks, etc. that were used to complete this project. Please do not use Excel for plotting. Use enough points in your lines so that the plots look as smooth as possible. You must properly cite any sources.

Organize your report to be in the format of a typical engineering resport with the following sections:

- Executive Summary: Briefly discuss the what you did and your major finding.
- Introduction: Discuss a brief introduction and background to this problem. Perform a very short lit review.
- Technical Approach: State the governing equations used for both the CV reactor and HCCI simulations and assumptions and governing equations for your model. If code was provided or downloaded, please state that. Do not derive the equations in this section. Instead, move the derivation into an Appendix.
- Code Verification: Discuss the limiting cases that were used to verify your model and the results. (Verification means that the equations are solved correctly.)
- Discussion and Results: Show and describe the results and general trends.
- Conclusions and Recommendations: Discuss the implications of the results, practical issues, inadequacies of the model, and potential model improvements.
- References
- Appendix: Details (such as derivations) that do not really belong in the body of a paper.

1 HCCI Engine Introduction and Basic Concepts

A Homogeneous Charge Compression Ignition (HCCI) engine is a relative new concept for reciprocating piston engines. The idea is to fill a combustion chamber with a uniform fuel-air mixture and then use compression heating to uniformly ignite the mixture. A HCCI engine can be idealized as a fixed mass reactor where the volume is changing as a known function of time, if the gas discharge processes through the intake and exhaust valves are neglected.

The cycles for an HCCI engine are shown in Fig. 1. Starting from Top Dead Center (TDC) the piston moves down while the intake valve is opened during the Intake Stroke, drawing a fuel-air mixture into the combustion chamber. Once the piston reactions Bottom Dead Center (BDC) the intake valve closes and the compression stroke begins where the fuel-air mixture is compressed. Once the fuel-air mixture becomes compressed enough as it reaches TDC for the second time, the entire mixture (hopefully) homogeneously autoignites without a spark plug. The high-temperature and combustion products push on the piston at is moves down from TDC to BDC during the power stroke. Once the piston has reached BDC the exhaust

valve opens and the combustion products exit the cylinder during the Exhaust Stroke. Finally the exhaust valve is closed when the piston reaches TDC. This cycle repeats itself every two revolutions (or four strokes). This is an overly-simplified description. The real scenario is much more complex and involves valve timings where they are not open and closed at exactly at TDC or BDC, there can be small lasers or weak sparks to control the ignition (as in the Mazda Skyactiv-X engine), cylinder gases can be pushed into the intake valve (sometimes intentionally in Miller cycle engines), heat transfer can quench combustion processes, etc.

In this project you will be modeling a simplified version of an HCCI engine. In your analysis you will

- Neglect friction and heat losses.
- The mixture in the engine is perfectly mixed and homogeneous at all times.
- Neglect any techniques to precisely control ignition. Ignition will occur through compression alone.
- Account for flow through the valves. However, assume that reverse flow through the valve does not occur. Assume that the enthalpy of the gas flowing through the valve is equal to the enthalpy of the reservoir where the gas is coming from. The "reservoir" for the fuel-air mix is at ambient conditions for the intake vales. The "reservoir" for the exhaust valve is instantaneous thermodynamic state in the cylinder.
- The engine is naturally aspirated (no turbochargers or superchargers) and draws in the fuel-air mixture at 300 K and 101325 Pa.

The work for a single engine cycle is

$$W = \oint P dV. \tag{1}$$

The average power (assuming the a four-stroke cycle engine) can be approximated by

$$\dot{W} = \frac{W}{2t_{\text{cycle}}} = \frac{WN}{120}, \tag{2}$$

where t_{cycle} is the time to complete one-full revolution of the engine. The torque can be computed based on the power:

$$\tau = \frac{\dot{W}}{2\pi N} \tag{3}$$

2 HCCI Geometrical and Mass Flow Relations

Some necessary geometrical relations are (assuming that the piston is not offset from the crank):

$$\dot{\Theta}(\text{rad/s}) = \frac{2\pi}{60} N \tag{4}$$

$$V(\Theta) = V_c + A_p \left[L + R + R\cos\theta - \sqrt{L^2 - (R^2 \sin^2 \Theta)} \right] \tag{5}$$

$$\frac{dV}{dt} = \dot{\Theta} A_p R \sin\Theta \left[-1 + \frac{R\cos\Theta}{\sqrt{L^2 - (R^2 \sin^2 \Theta)}} \right], \tag{6}$$

where N is the engine rotation speed in RPM, V_c is the clearance volume which is the gas volume when the engine is at Top Dead Center (TDC) ($\Theta = 0°$), A_p is the piston area given by $A_p = (\pi/4)B^2$, L is the length of the connecting rod, R is the length of the crank arm, and B is bore (diameter of the piston). The piston is said to be at Bottom Dead Center (BDC) if the volume is maximized ($\Theta = 180°$).

The clearance volume can be computed from a given stroke length ($S = 2R$), bore, and compression ratio, Cr is

$$V_c = V_d/(Cr - 1); \quad V_d = SA_p, \tag{7}$$

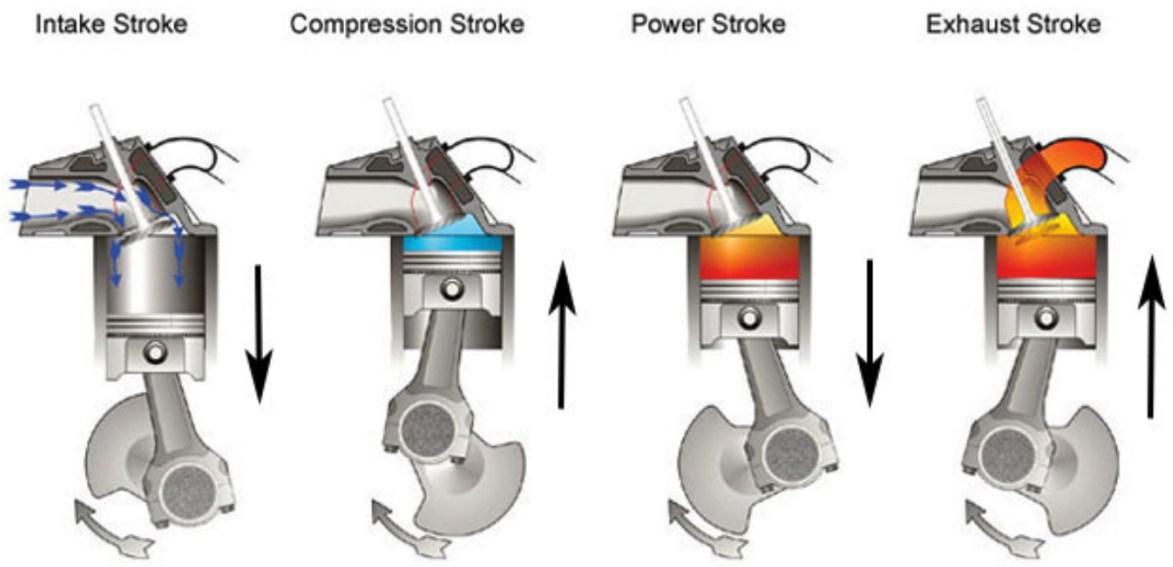

Figure 1: Cycles in a HCCI engine

where V_d is the displacement volume. The volume at Bottom Dead Center (BDC) is $V(180) = V_c + V_d$, and volume at TDC is $V(0^\circ) = V_c$.

In this project you will be assuming that the combustion chamber is perfectly insulated, but will include the effect of the intake and exhaust valves. The mass flow rate flowing through a valve is

$$\dot{m} = A_{valve} C_d \dot{m}'', \tag{8}$$

where A_{valve} is the instantaneous valve area, C_d is the discharge coefficient (assume for this project that $C_d = 1$) and $\dot{m}''$ is the mass flux through the valve. The mass flux is given by

$$\dot{m}'' = \frac{p_o}{\sqrt{RT_o}} \Gamma(M, \gamma), \tag{9}$$

where p_o is the stagnation pressure in the reservoir driving the flow through the valve, T_o is the stagnation temperature upstream of the valve, γ is the ratio of specific heats based on the local gas mixture flowing through the valve,

$$\Gamma(M, \gamma) = M\sqrt{\gamma}\left[1 + \frac{\gamma - 1}{2} M^2\right]^{\frac{\gamma+1}{2(\gamma-1)}}, \tag{10}$$

M is the Mach number of the flow through the valve (modeled as an oriface)

$$M = \min\left[1, \sqrt{\frac{2\max\left[\left(\frac{p_o}{p_b}\right)^{\frac{\gamma-1}{\gamma}} - 1, 0\right]}{\gamma - 1}}\right], \tag{11}$$

and p_b is back pressure down stream of the valve. Assume that the engine is naturally aspirated (pulls in air at atmospheric pressure without a supercharger or turbocharger) with $p_{ambient} = 101325$ Pa and $T_{ambient} = 300$ K. You may assume that exhaust flows into the ambient air. *Hint: The stagnation and back pressures are "flipped" between the exhaust the intake valves.* You may assume that reversed flow is not possible with the valve, meaning that cylinder gases will not be pushed out through the intake valve.

The valves to not instantly open or close. In this project, we simplify the valve opening and closing using *tanh* functions, which can be used to construct smeared step functions. The code below can be used to calculate the instantaneous valve areas:

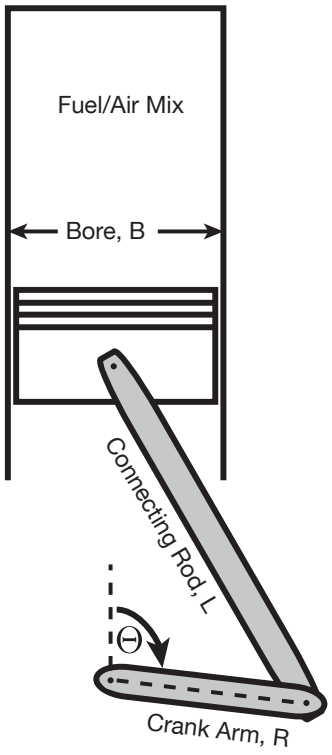

Figure 2

```
def intake_valve_area(self, theta):
theta_shift = 360.
t = (theta + theta_shift)%720
to_rel = self.intake_open_angle + theta_shift
tc_rel = self.intake_close_angle + theta_shift

y = self.intake_max_area*0.5*(
np.tanh((t - to_rel)/self.intake_rise_factor) -
np.tanh((t - tc_rel)/self.intake_rise_factor))
return y

def exhaust_valve_area(self, theta):
theta_shift = 360.
t = (theta + theta_shift)%720
to_rel = self.exhaust_open_angle - theta_shift
tc_rel = self.exhaust_close_angle - theta_shift

y = self.exhaust_max_area*0.5*(
np.tanh((t - to_rel)/self.exhaust_rise_factor) -
np.tanh((t - tc_rel)/self.exhaust_rise_factor))
return y
```

Here the opening and closing angles are the crank angles (in degrees) where the valves are opened to 50% of their maximum value. The rise factors control how fast the valves open. A tiny rise factor will open and close the valves very rapidly. A large rise factor will open and close the valve very slowly. The maximum intake and exhaust areas are the flow areas for the valves if the valve is fully opened. The flow area for the intake valve is an annular region with an outer diameter (the intake port diameter) of $0.45B$ and an inner

Table 1: Engine parameters

Parameter	Value
L	145.54 mm
B	82.0 mm
S	90.4 mm
Cr	90.7 mm
N (RPM)	varies
Intake Mixture	varies
T_{intake}	300 K
p_{intake}	101325 Pa
Intake Port Diameter	$0.45B$
Exhaust Port Diameter	$0.37B$
Valve Stem Diameter	$0.25B$
Number of Intake Valves	2
Number of Exhaust Valves	2
Intake Valve Rise Factor	20
Exhaust Valve Rise Factor	20
Intake Openening Angle	0°
Intake Closing Angle	220°
Exhaust Openening Angle	540°
Exhaust Closing Angle	720°

diameter (accounting for the valve stem) of $0.25B$. The flow area for the exhaust valves is an annular region with an outer diameter (exhaust port diameter) of $0.37B$ and an inner diameter (accounting for the valve stem) of $0.25B$. There are 2 exhaust valves and 2 intake valves.

The parameters for the engine that you are modeling are given in Table 1. The intake and exhaust valve area as a function of θ for these parameters are shown in Fig. 3

3 Problems

In this project we will work towards modeling a Homogenous Charge Compression Ignition (HCCI) engine that is operating with a realistic primary reference fuel (PRF) that contains a blend of iso-octane and n-heptane. The steps of this project are

1. Download a reaction mechanism for a realistic fuel to be used for your HCCI simulations and convert it to Cantera format (yaml or cti).

2. Run the supplied python code for a constant-volume reactor adiabatic reactor.

3. Use a control volume analysis to derive governing differential equations for the HCCI which has time-varying volume and mass flow through valves.

4. Modify the constant-volume reactor code to solve the HCCI equations and verify that the various pieces are working properly.

5. Run the model for selected cases.

More information for each of these steps is provided below.

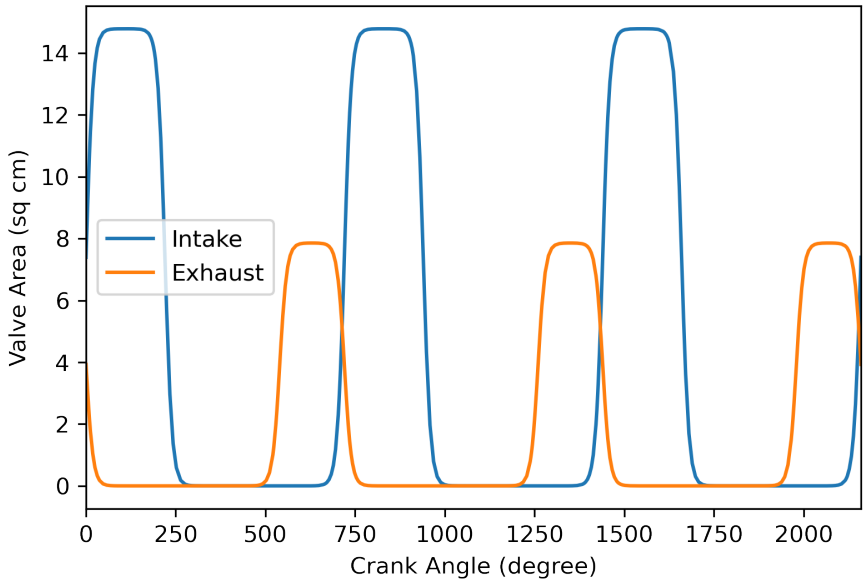

Figure 3

3.1 Step 1 - Obtain a Cantera File for Realistic Fuel

Thermodynamic, chemical reaction, and transport data files are often available in Chemkin format, but not Cantera. These files can be converted Cantera input using `ck2yaml` or `ck2yaml.py`, which comes with Cantera. Please see https://cantera.org/tutorials/input-files.html for more information.

There are a wide variety of sources for the chemical reaction mechanism files including

- Full chemical reaction mechanisms, such as those made available by the combustion group at Lawrence Livermore National Laboratory (LLNL) https://combustion.llnl.gov/mechanisms
- Reduced chemical models (using SS, PEA, and other techniques) and skeletal mechanisms (some species and reactions are "deleted" from the full mechanism) for realisitic fuels from Prof. Tianfeng Lu's grroup at the University of Connecticut: http://spark.engr.uconn.edu/mechs/mechs.htm
- The Chemical Kinetics Laboratory at USC led by Prof. Hai Wang (now at Stanford) http://ignis.usc.edu/research.html, which contains USC MechII.
- The HyChem database, developed by Prof. Hai Wang at Stanford, has detailed reaction mechanisms for realistic jet fuels, rocket fuels, and gasoline https://web.stanford.edu/group/haiwanglab/HyChem/pages/download_cantera.html .
- The Soot reaction mecanism of Appel, Bockhorn, and Frenklach at UC Berkeley, http://combustion.berkeley.edu/soot/mechanisms/abf.html.
- Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS), which contains many chemical reaction mechanisms in Cantera Format. https://www.cerfacs.fr/cantera/mechanisms/meth.php#
- The University of California San Diego also has a group developed chemical reactio mechanisms. http://web.eng.ucsd.edu/mae/groups/combustion/mechanism.html.
- Many journal papers with detailed chemical reaction mechanisms will often have mechanism files posted in the supplemental material. For example, the mechanism of Cai and Pitsch (2015) is available as supplemental material from Cai and Pitsch, *Combustion and Flame*, (2015), Vol. 162, pp. 1623-1637.

Download the Chemkin files for the 171-species skeletal mechanism for the PRF blend of iso-octane and n-heptane from Prof. Lu's website. Convert these Chemkin files to a cantera `cti` file.

3.2 Step 2 - Run the Constant-Volume Reactor Code

Use the functions in the `Chemical_Kinetics_and_Reactors.ipynb` notebook supplied on the Canvas website to integrate a constant-volume reactor and to find the ignition delay times. Specifically,

a) Plot the ignition delay time for PRF-0, PRF-50, and PRF-100 mixtures at a pressure of 40 atm and an equivalence ratio of 0.3 as a function of reactant temperature ranging from 600 to 1500 K. Use a log-scale for the y-axis. Comment on the definition of the ignition delay time used in the code. Use at least 100 points for each plot.

(PRF-X fuel is a blend of n-heptane (`NC7H16`) and iso-octane (`IC8H18`), where X is the mole fraction of n-heptane on a percent bases. For example, PRF-75 fuel consists of 25% iso-octane and 75% n-heptane on a molar basis).

Note: The Octane Number for a PRF fuel is defined as blending ratio between iso-octane (Octane number of 100) and n-heptane (Octane number of 0). The Octane number really represents the resistance of a fuel to autoignite under compressure. Measureing the octane number is difficult for a real fuel and different methods produce different results. Generally, the fuel is tested in an engine at precisely controlled conditions, and comparing the results of the real fuel and comparing with blends of iso-octane and n-heptane. Thus, because we are precisely controlling the amount of iso-octane and n-heptane, the Octane number of the blended PRF-X fuel is $100 - X$.

b) Plot the temperature and pressure as a function of time (on a log scale for the x-axis) for PRF-50 mixtures at an equivalence ratio of 0.3, a pressure of 40 atm and temperatures of 775K, 1225K, and 1700K.

c) Pick an interesting case from part b) and plot the mass fractions of n-heptane, iso-octane, O_2, CO_2, H_2O, CO, OH, H, CH_3, and H_2O_2 on the one y-axis as a function of time (log-log scale) and the chemical energy release rate on a second y-axis.

d) Plot the ignition delay time for PRF-100 at an equivalence ratio of 0.3 at pressures of 5, 10, and 40 atm for temperatures ranging from 600 to 1500K. Comment on the influence of pressure on the ignition delay time.

3.3 Step 3 - Derive Governing ODEs for an HCCI Engine

Derive a set of differential equations that can be used to model an idealized HCCI engine as a fixed-mass reactor, but with volume changing as a prescribed function of time. Take heat transfer through the walls into account. Show your control volume(s). Your final governing equations should be for ρ, T, and Y_i.

The equations will be simpler if you perform a change of variables an solve then as $d()/d\theta$ rather than $d()/dt$

3.4 Step 4 - Modify the Constant-Volume Reactor Code to Solve the HCCI ODEs

Modify the example functions for the constant-volume fraction to solve the equations that you derived for the HCCI engine. In addition, write functions to compute the power and torque output for this engine for one full cycle (720°). Note: You will have to average the results over many cycles (say 20) to get a reasonable average for some cases.

Verify that the components of your model are working correctly by turning various terms on and off and compare to analytical solutions or known codes that work. Specifically:

1. Set the maximum valve areas to zero and force dV/dt to be zero (or nearly zero at the very least). This should setup the limiting case of a constant-volume adiabatic reactor, but solving the model equations

for the HCCI engine. Repeat one of the calculations from the constant volume reactor using the HCCI engine model with $A_{valve} = 0$ and $dV/dt = 0$. Compare the temperature vs time for both reactors on the same figure. They should overlap with very little difference.

2. Set the maximum valve area to 0 and pick a gas mixture that has no chemical reactions and *constant* specific heat, but allow the volume to change as a function of time. (What type of species has constant C_p?) The energy equation should reduce to a very special case under these conditions with a very simple exact solution for the temperature and pressure as a function of volume. Derive this (very familiar) expression from the energy equation under the limiting case of zero heat transfer and constant specific heat. Compare the computed temperature and pressure to the exact equation.

3.5 Step 5 - Run the HCCI Model

Now run the model. You will have to use a stiff ODE solver (BDF) usually works fine with some fairly tight error tolerances. Relative and absolute error tolerances of 10^{-8} and 10^{-10} work well, but you will have to experiment.

Some cases will have cycle-to-cycle variations. Run the models for at least 30 cycles and average the torque and power output for at least 20 cycles.

1. Run the HCCI model for PRF-50 at $\phi = 1$ with engine speeds of 2500 and 5000 RPM. Plot the pressure, temperature, and some species as a function of θ for one *complete* cycle. Note: A *complete* cycle may be 720°, 1440°, 2160°, or 2800°, depending on the variations that occur. In addition, make a P-V diagram for these two cases and find interesting and qualitatively compare with the Otto cycle.

   In your report comment why the 5000 RPM case is not desirable.

   Note: This is a fairly complex model may take awhile to run. Some cases take 10 minutes on my laptop.

2. Run four series of three simulations using PRF-25, PRF-50, and PRF-75 with engine speeds ranging from 500 to 8000 RPM. Plot the torque produced by the engine for all three series on a single plot and plot the power (in HP) produced by engine on a single plot. Comment on the common assumption in the hot-rod and racing communities that "higher octane number always means more power".

3. (EML 5131 Students Only) The mass specific emission (MSE) is defined as

$$MSE = \frac{\text{Mass flow rate of pollutant}}{\text{Power Produced}} = \frac{\text{Mass of pollutant}}{\text{Work Output}}. \tag{12}$$

   The effiency, η, is defined as

$$\eta = \frac{\text{Chemical energy in}}{\text{Work Out}} = \frac{m_f LHV}{W}, \tag{13}$$

   where m_f is the mass of the fuel that enters the combustion chamber during a complete cycle. Plot MSE for CO and the efficiency for each of these cases as a function of engine speed. *Hint: The mass of the fuel and mass of the CO leaving the engine can be computed using the computed solution by integrating $Y_i \dot{m}$ through the valves where i is CO for MSE and i is the fuel mixture for the efficiency.*