Application Note: CHEMKIN / CHEMKIN-PRO

Single Zone Homogeneous Charge Compression Ignition (HCCI) Engine

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Summary

Homogeneous Charge Compression Ignition, or HCCI, is an advanced combustion technology for internal combustion engines. The main appeal of the HCCI engine is the great potential for lowering emissions and improving fuel economy.

Project Description

For this application, we have ignition data from a single-cylinder HCCI test engine and would like to use the single-zone IC engine model to simulate the same HCCI process. We would also like to find out how sensitive the solutions are to the assumed heat loss at the cylinder wall.

The HCCI engine for this example runs on natural gas, a mixture of CH_4, C_2H_6 and C_3H_8, with exhaust gas recirculation (EGR). Using EGR increases the reliability of ignition under a wider range of operating conditions. Additionally, CO_2 from the exhaust gas can keep combustion temperatures low, due to its relatively large heat capacity. Specifications of the test engine that are related to our model setup are given in Table 1.

Table 1 Test Engine Specifications

Parameter	***Setting***
Compression ratio	16.5
Cylinder clearance volume	103.3 cm^3
Engine speed	1000 rpm
Connecting rod to crank radius ratio	3.714286
Cylinder bore diameter	12.065 cm

Problem Setup

CHEMKIN-PRO provides a pre-defined reactor model for HCCI engine simulations. The model is called the Closed Internal Combustion Engine Simulator it from the Models Palette (see Figure 1).

Figure 1 Closed Internal Combustion Engine Icon

The next step is to define the chemistry set, or combustion mechanism, for our HCCI simulation. Since methane is the main component of natural gas, the mechanism we have selected is the GRI Mech 3.0 to describe the combustion process and use methane as the “surrogate” fuel. After pre-processing the mechanism data, we specify the engine parameters in the Reactor Properties panel.

The IC Engine model is appropriate for a closed system, representing the time between intake-valve closure and exhaust-valve opening in the engine cycle. The start time (or start crank angle) therefore represents the time of intake-valve closure. As a convention, engine events are expressed in crank rotation angle relative to the top dead center (TDC). The intake valve close (IVC) time of our test engine is 142 degrees (crank angle) before TDC (BTDC). Because the GUI requires input as the crank angle after TDC, we should set our simulation starting crank angle to –142 degrees (ATDC). We let the simulation run for 257 crank angle degrees to 115 degrees (ATDC). The gas mixture pressure and temperature at IVC are 107911 Pa (or 1.065 atm) and 447 K, respectively. The composition of the initial gas mixture is a combination of natural gas, air, and EGR gas and is given in Table 2.

Table 2 Composition of Initial Gas Mixture

Species	***Mole Fraction***
CH_4	0.0350
C_2H_6	0.0018
C_3H_8	0.0012
O_2	0.1824
CO_2	0.0326
H_2O	0.0609
N_2	0.6861

There are two different approaches to defining the heat loss through the cylinder wall. One approach assumes the cylinder is adiabatic and the other considers heat loss through the cylinder wall.

Parameters that describe heat transfer between the gas mixture and the cylinder wall are specified on the Reactor Physical Properties panel. For the non-adiabatic conditions, we have several ways to describe the heat loss to the wall: a constant heat transfer rate (where a positive value corresponds to heat loss from the gas to the environment), a piecewise-linear heat-transfer-rate profile, a user-defined subroutine, or a heat-transfer correlation specifically designed for engine cylinders. Here we choose the heat-transfer correlation for our HCCI problem. In this example we also apply the Woschni correlation[1] to get better estimates of gas velocity inside the cylinder.

Project Results

After successfully running both adiabatic and heat-transfer-correlation IC Engine projects, we can launch the CHEMKIN-PRO Post-Processor from the Analyze Results panel of one the projects. We can load the solutions from the other project by using the **File > Open Solution File** option of the Post-Processor Control Panel.

The temperature solutions are shown in Figure 2. Again, a crank-rotation angle of 0 degrees corresponds to TDC. We notice that the measured gas temperature before ignition is higher than the one predicted by the adiabatic model. If the measurement was done correctly, this could mean that a small portion of fuel starts burning before TDC and our model fails to capture this phenomenon. The ignition time predicted by the adiabatic model is about 5 degrees earlier than those obtained by experiment and by the non-adiabatic model. The temperature solution from the non-adiabatic model generally agrees with the measurement. Both models predict stronger ignition in the cylinder as indicated by the sharp increases in the temperature profiles. The weaker ignition shown by the experimental data is likely due to temperature variation inside the real cylinder. Although gas composition is homogeneous throughout the cylinder, gas temperature in the core region can be different from that in the boundary layer. The temperature difference can be large if heat loss at the cylinder wall is large. If the gas mixture of the hot core region ignites first, the mean temperature inside the cylinder will not jump as sharply as predicted by the models.

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[1] J. B. Heywood, *Internal Combustion Engines Fundamentals*, McGraw-Hill Science/Engineering/Math, New York, 1988.

Figure 2 HCCI Engine—EGR Temperature Comparison

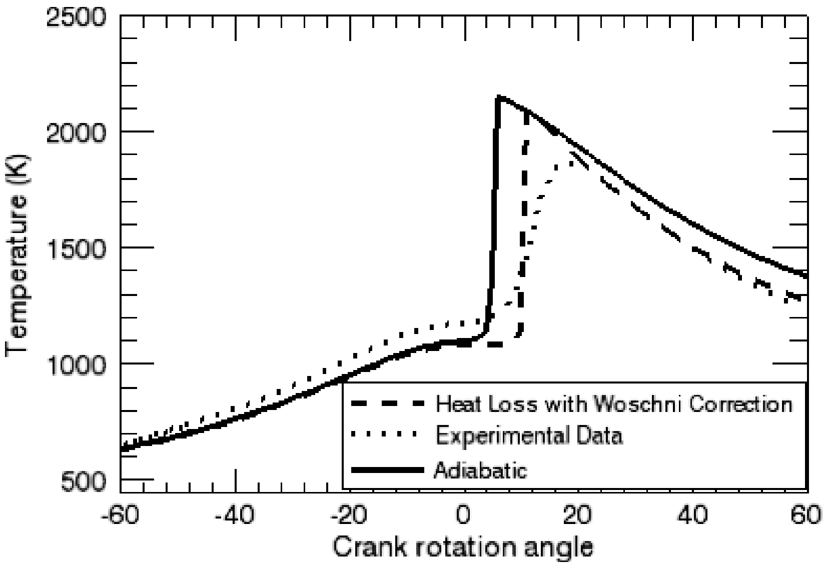
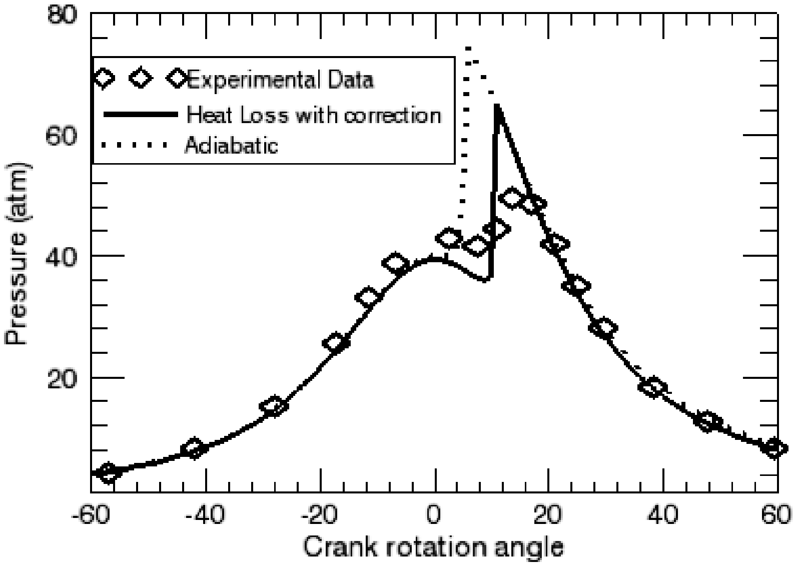


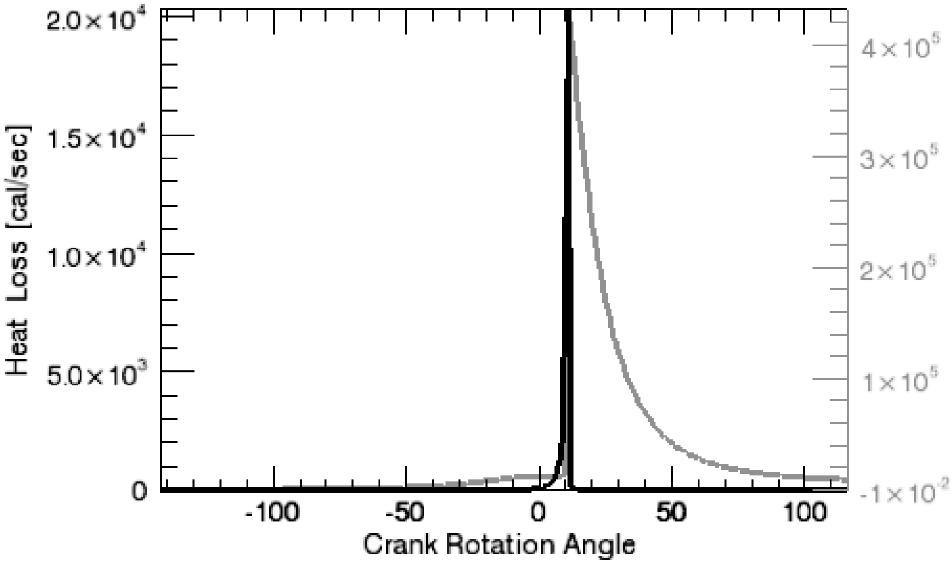
Figure 3 gives the comparisons of the measurement and the predictions. In general, the profiles show similar trends as observed in the temperature profiles except that the pressure results are less sensitive to heat loss.

Figure 3 HCCI Engine—EGR Pressure Comparison



We can examine the heat-release rate profile for the timing and the magnitude of heat generated by combustion. Since the temperature profile predicted by the non-adiabatic model is in good agreement with the measurement, we can determine how much thermal energy is dissipated to the environment, i.e., the heat loss rate, during the combustion/expansion period. The heat-release rate and the heat loss rate profiles predicted by the non-adiabatic model are shown in Figure 4. Note that the heat-release profile typically contains narrow spikes. If we want to calculate the total heat-release from the heat release rate profile, we must make sure the profile has enough time resolution to reduce numerical error.

Figure 4 HCCI Engine—EGR Heat Loss Comparison



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