Modeling HCCI Engine with Exhaust Gas Recirculation

PRO-APP-Auto-7 (v2.0) August 30, 2010

Overview

Exhaust Gas Recirculation (EGR) in an engine serves to limit the generation of NO_x during in-cylinder combustion. This application note demonstrates the use of a Reactor Network to determine the initial gas composition in an HCCI Engine with Exhaust Gas Recirculation.

Introduction

Homogeneous charged compression ignition (HCCI) engines are receiving renewed attention and enthusiasm in the automotive industry. HCCI engines can be controlled to produce low emissions while achieving engine efficiency comparable to diesel engines. These engines have been shown to generate very low levels of nitrogen oxide emissions (NOx) without the use of an aftertreatment catalytic converter.

One of the strategies to control ignition in an HCCI engine is to charge the cylinder with a mixture of exhaust gas and fresh fuel-air mixture. The introduction of exhaust gas impacts ignition in several ways. Thermodynamically, the added exhaust gas could increase the initial gas temperature and affect gas temperature during compression by modifying the mixture‘s specific-heat capacity. The presence of exhaust gas also influences ignition kinetics through a dilution effect and through introduction of alternative reaction pathways such as NO_x-mutual sensitization.

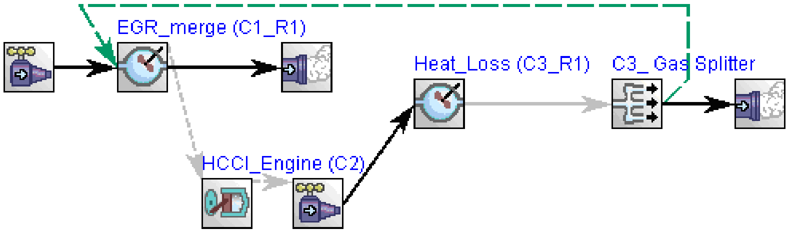
This application note describes the use of CHEMKIN-PRO's HCCI engine model, along with a tear stream connection in a reactor network, in order to simulate an HCCI+EGR system. Since the composition and temperature of a recycled exhaust-gas mixture are part of the solution to the HCCI engine model, they are not known prior to running the simulation. The tear-stream iterative solution allows the user to determine exhaust-gas properties by running the simulation iteratively. This iterative scheme will converge when the initial gas properties inside the cylinder do not show significant cycle-to-cycle variations.

This approach to engine modeling could be employed to build correlations between intake gas properties, engine operating conditions, EGR ratio, and exhaust-gas conditions, and to map a “stable” HCCI engine operation regime in terms of EGR ratio, engine speed, fuel equivalence ratio, and fuel type.

Running an HCCI Engine Model with EGR

Here we discuss an example of an HCCI-EGR network project, in which there are three computational components to the simulation, as shown in the diagram view below. The HCCI Engine cluster (C1) represents the HCCI engine cylinder, of which the initial condition at intake valve closure (IVC) is not known *a priori*, due to the presence of external EGR. The Heat_Loss (C3) cluster is a simplified model of the collection of pipes and valves that circulates exhaust gas back to the intake manifold. This example assumes 30% of the exhaust-gas mass gets recycled. Chemical reactions and heat transfer are allowed in the EGR pipe system. The cluster labeled EGR_merge (C1) simulates the blending of the fresh fuel-air mixture and the recycled exhaust gas in the intake manifold. The green dashed line in the diagram view of the EGR network project represents the recycle stream. The simulation is converged when the properties of this recycle stream no longer change from one iteration to the next, within user-defined tolerances.

Figure 1. Diagram view of the EGR network project.



The EGR_merge reactor performs the mixing between the fresh fuel-air mixture and the recycled exhaust gas. In this project, an open PSR model is used for this purpose, so that chemical reactions are allowed to take place as soon as the gases are mixed; alternatively, a Gas Mixer could also be employed here. The reactor pressure during mixing is specified to be the same as the in-cylinder pressure of the HCCI engine at IVC.

Parameters and operating conditions of the HCCI engine are entered in the corresponding Reactor Properties panel in the CHEMKIN-PRO Interface. Initial gas temperature, pressure, and composition are not needed here as they will be obtained directly from the solution of the EGR_merge reactor.

The main purpose of the Heat Loss reactor is to capture the cool down of the hot exhaust gas that may occur as it travels from the exhaust valve to the intake. It is important to provide suitable values for residence time, heat transfer coefficient, internal surface area, and ambient temperature that represent the actual geometry and heat-transfer environment of the engine. The solution from the HCCI engine simulation will supply the temperature and composition of the inlet mixture.

The specified values of mass flow rate for the Heat_Loss reactor and the EGR_merge reactors determine the EGR ratio between the recycled exhaust gas and the fresh fuel-air mixture. In this case, the Heat_Loss reactor has a mass flow rate of 10 g/sec and the targeted ratio is 0.3. Therefore the mass flow rate of the recycled exhaust gas is set to 3 g/sec. Since the mass flow rate of fresh fuel-air mixture to the EGR_merge reactor is 7 g/sec, the mass ratio of the fresh fuel-air mixture and exhaust gas is 7:3 or 30% EGR by mass. After the project has been set up, it is run like other CHEMKIN-PRO projects through the **Run Calculations** node on the Project Tree.

After running, the user can take a look at the HCCI engine solution in the Graphical Post-Processor. Plots comparing "steady state" results of the current HCCI Engine simulation (30% EGR) and those without EGR are given in the following set of plots, Figure 2 through Figure 5.

Figure 2. Comparison of EGR effect on in-cylinder pressure. Solid line: no EGR; Dash-dotted line: 30% EGR by mass.

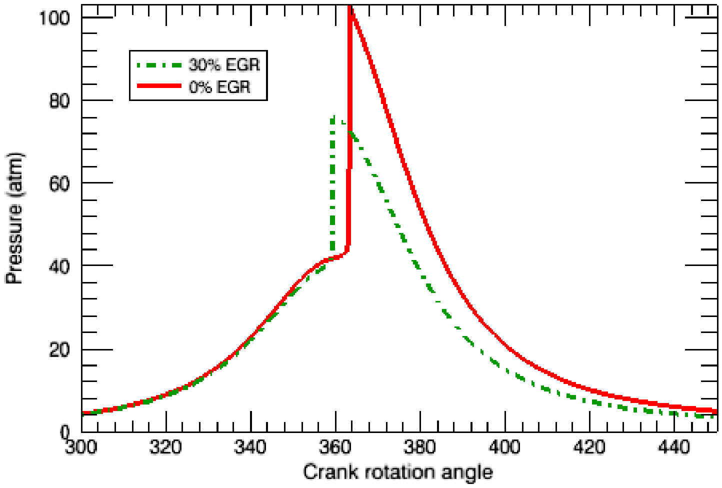


Figure 3. Comparison of EGR effect on gas temperature. Solid line: no EGR; Dash-dotted line: 30% EGR by mass.

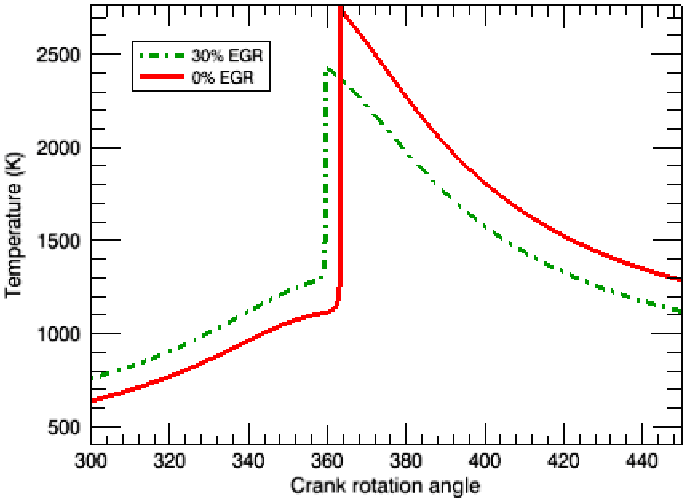


Figure 4. Comparison of EGR effect on CO_2 emission. Solid line: no EGR; Dash-dotted line: 30% EGR by mass.

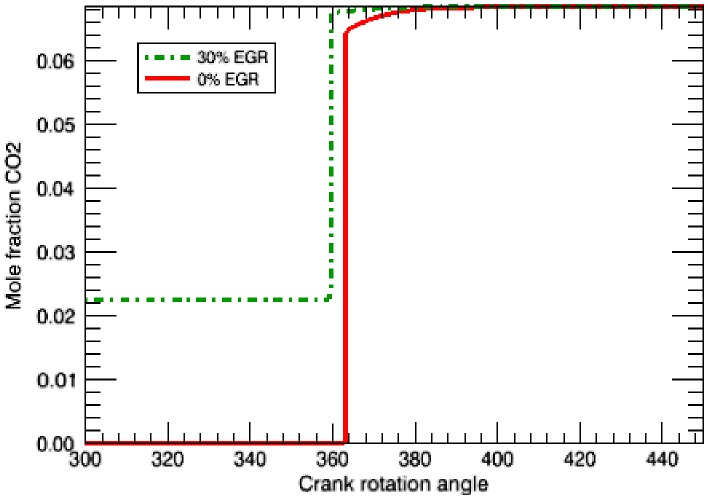
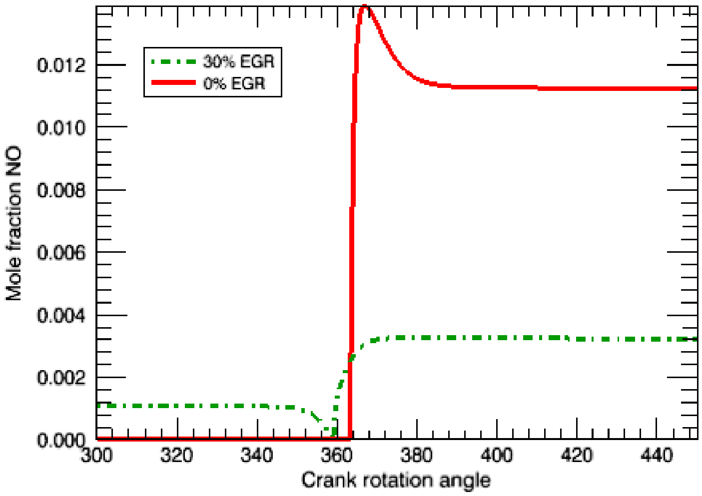


Figure 5. Comparison of EGR effect on NO emission. Solid line: no EGR; Dash-dotted line: 30% EGR by mass.



Summary

Determining the effects of EGR on HCCI engine operation is just one of many automotive applications that can be modeled with CHEMKIN-PRO's HCCI Combustion Model. For the user needing more accurate emission results, the Multi-zone model allows specifying non-uniform initial conditions and heat transfer for regions within the cylinder. To see more uses of the Multi-zone model, please see the Multi-Zone Engine Model Application Note. To see how more intricate Reactor Networks can be built and applied in CHEMKIN-PRO, refer to our extensive collection of application notes.

All of these materials and much more can be found on our website at www.reactiondesign.com. If you have any questions about this application note or about any of our products or services, please do not hesitate to contact our sales or technical teams at sales@reactiondesign.com or support@reactiondesign.com.

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