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Dual-Fuel Homogeneous Charge Compression Ignition Engine with Ethanol and 1-Octanol

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Abstract - Due to stricter regulations on exhaust gas emissions in the upcoming Euro 7 emission norms, a deeper onus is put upon developing alternative combustion concepts with renewable fuels, thus increasing the overall internal combustion engine (ICE) efficiency and reducing exhaust emissions. As a part of the Munich Mobility Research Campus (MORE) Project, a serial hybrid vehicle is being developed based on a dual-fuel homogeneous charge compression ignition (HCCI) engine concept operating on a less reactive port-injected fuel of ethanol with a more reactive direct-injected fuel of 1-octanol. The current concept involves injecting 1-octanol early at the end of the intake stroke, so that the mixture formed is highly homogeneous, resulting in extremely low soot emissions, as opposed to a reactivity-controlled compression ignition (RCCI) concept, where the high reactivity fuel is injected shortly before ignition. This paper deals with developing a methodology to simulate the combustion concept for optimizing the boundary operation conditions, such as intake temperature, valve timing, injected amount, etc. Simulation models in 0-D, 1-D and 3-D with computational fluid dynamics (CFD) are developed using ANSYS Chemkin, GT Power, and AVL Fire M software, respectively, integrating a reduced chemical kinetic mechanism. The cylinder pressure curves and heat release characteristics from the simulation model will be validated against testbench measurements for a stable operating point. These validated models will form a baseline for the simulations, which would be further used in optimizing the parameters, such as valve timing, injection quantity, and timing, intake temperature, pressure, etc., for the other application operation points on the serial hybrid powertrain.

***Keywords*:** Low Temperature Combustion, Dual Fuel HCCI, RCCI, Ethanol, 1-Octanol, Simulation, Chemical Kinetics

1. Introduction

In order to conform with the Euro 7 emission norms, future engine development must involve research with renewable fuels and highly efficient and ultra-low engine emission processes. In comparison to gasoline engines and diesel engines, the homogeneous charge compression ignition (HCCI) concept provides advantages of higher efficiency due to higher compression ratio and lean mixtures used, and lower emissions of soot and NO_x due to homogeneous and lean mixtures and lower combustion temperatures. The inherent difficulty with HCCI concepts is the combustion phasing and controllability, higher rate of heat release, and combustion noise. To improve the combustion phasing and controllability, temperature and fuel stratifications are developed like partially premixed compression ignition (PPCI), spark-assisted compression ignition (SACI), reactivity-controlled compression ignition (RCCI), etc. All these combustion concepts are grouped under low-temperature combustion (LTC) or controlled auto-ignition process (CAI). Various studies, such as [1], have focused on the effect of control parameters and their effects on the resulting efficiency and emissions in LTC. Using spatial fuel stratification and reactivity stratification, through the RCCI combustion process, increase of gross indicated efficiency of 16.4 % is shown in [2]. From all these literatures, it is clear to identify the potential of the RCCI concept in a standalone or a hybridized powertrain concept to tap the advantages of the combustion process and also to use a phlegmatized and optimized powertrain.

In addition to using an alternative combustion process, there are many advantages in using renewable and sustainable fuels. The advantages of using and manufacturing ethanol are already well studied. Ethanol is already used as a major replacement of gasoline and shows its advantages in reducing the NO_x and soot emissions have been demonstrated [3]. 1-Octanol is a promising candidate to replace diesel due to its similar characteristics to diesel along with lower soot emissions due to its oxygen content. 1-Octanol as a CO_2 neutral fuel for commercial vehicles is studied in [4].

The goal of the Munich Mobility Research Campus Project (MORE) at the Universität der Bundeswehr, München is the holistic demonstration of a sustainable and environmentally friendly mobility solution. As a part of the powertrain

development sub-project, a highly phlegmatized serial hybrid powertrain is being developed using the proposed dual fuel HCCI engine with alternative fuels [5]. Due to the aforementioned advantages of renewable fuels, ethanol was chosen as the low-reactivity fuel and octanol was chosen as the high-reactivity fuel. To validate the concept, simulation of the engine plays a vital role. This paper presents a method for validation of the concept with the help of 0-D, 1-D and 3-D CFD simulations. In the first section, the challenges of the concept and simulation methodology are discussed. Subsequently, the model development for each of the simulation types is presented. Finally, future steps for the validation of the models on the test bench and the baseline results from the simulation are proposed.

2. Proposed Concept and Challenges

The dual-fuel HCCI concept is like the RCCI combustion concept, except that the spatial fuel stratification has been eliminated and the controllability is achieved only through the variation of the relative concentration of fuels with different reactivity. The early injection of the high-reactivity fuel results in a homogeneous mixture preparation and lower soot emissions. Hence it can be considered a dual-fuel HCCI concept and is depicted in Figure 1.

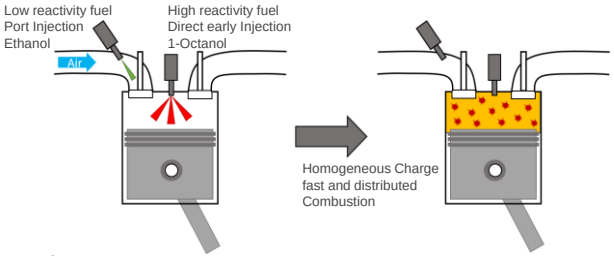

Fig. 1: Proposed dual-fuel homogeneous charge compression ignition combustion concept

The intake-port-injected low-reactivity fuel (ethanol) is injected very early in the intake phase to enable better mixture formation. Pre-heating and boosting the engine are necessary to achieve autoignition due to fact that the heat of vaporization of ethanol is evidently higher than gasoline and this results in the cooling of the mixture. The high reactivity fuel (1-octanol) is injected by direct injection, but very early (-200°CA bTDC). For faster combustion control and combustion phasing, the amount of the injected high-reactivity fuel will be the control variable.

The number of operating parameters for the proposed concept is also higher than the conventional combustion engines, as various parameters, like injected fuel reactivity, quantity, injection timing, required air mass, boost pressure, intake temperature, rest gas content in the engine, valve timing, compression ratios, piston geometry, intake and exhaust port design for the mixture movement, cooling system boundaries for initiating autoignition and some more auxiliary systems, influence the ignition. Due to the complexity of the optimization problem, simulation models are necessary to design the auxiliary systems and to refine the combustion process for achieving higher efficiency and lower emissions.

3. Simulation methods

Currently, no empirical models exist, that the HCCI or dual fuel combustion, or RCCI satisfactorily simulates. This necessitates the development of a new simulation concept for this innovative combustion process. The aforementioned 0-D, 1-D and 3-D simulation models, each based on chemical kinetics, are developed to simulate specific components in the engine system, as shown in Figure 2. The 0-D simulation is used to investigate the auto-ignition conditions and the general combustion behavior of the fuels used. The 1-D system simulation of the engine and its auxiliary components is carried out to design the auxiliary systems and to determine the optimal parameters at the start of compression to achieve the auto-ignition conditions and to increase the system efficiency. The optimized parameters are used in the 3-D CFD simulation of the combustion chamber to obtain a clear understanding of the mixture flow and the combustion processes. To validate the simulation results, an existing single-cylinder research engine is converted for dual-fuel operation. The experimental results from the dual fuel HCCI operation, like the cylinder pressure curve, the heat release rate, and the exhaust gas composition, are used for comparison to the simulation results.

3.1. Chemical kinetic mechanism

As the process depends heavily on the reactivities of both fuels, the simulation models incorporate a chemical kinetic mechanism. In cooperation with ITV, RWTH Aachen, a new reduced mechanism with ethanol and 1-octanol based on the detailed mechanism from [6] is being developed and validated for 3-D CFD simulations and will be applied in all the simulation models. . The mechanism will also include a reduced NO_x mechanism based on Lamoureux [7] to estimate the NO_x emission from the LTC.

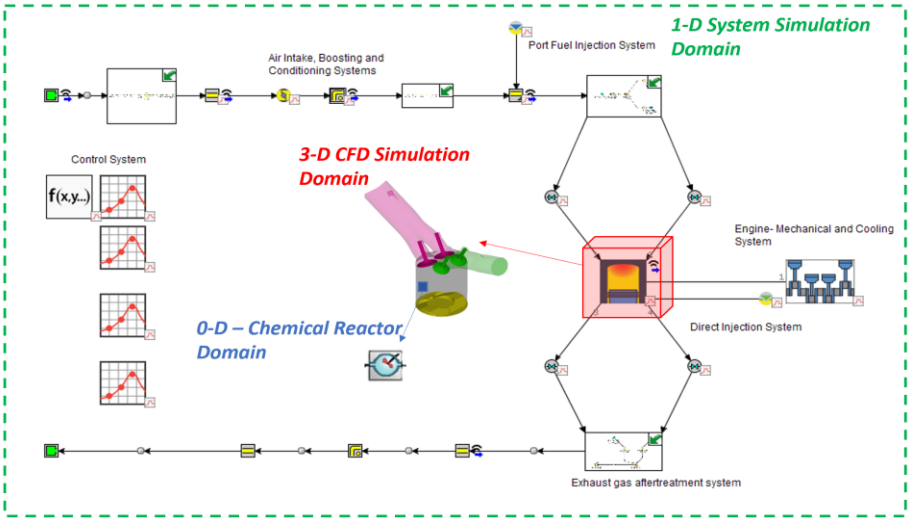

Fig.2: Definition of 0-D chemical simulation, 1-D system simulation and 3-D CFD simulation domains

3.2. 0-D Combustion Simulation

For the 0-D combustion simulation, ANSYS Chemkin was used. As the mixture of air with ethanol and 1-octanol in the present concept is considered homogeneous, the HCCI model in Chemkin is used, which includes a homogeneous chemical reactor. The vaporization, spatial inhomogeneities of fuel (specifically direct injected 1-octanol) and temperature, and heat loss due to vaporization is not considered in the 0-D simulation. The homogeneous reactor simulates the basic state of the mixture at various temperature and pressure points in the engine cycle, calculated using the piston movement equations. The 0-D simulation needs the basic geometry information of the engine (to simulate the volume change), intake temperature, pressure and composition of the mixture at the start of the compression phase. The start of compression in the simulation is the intake valve closing crank angle and the end of the expansion is the exhaust valve opening crank angle and the chemical simulation is carried out only between these events. The heat loss model is calibrated with the help of the model coefficients. From this simulation, immediate results of the indicated pressure curve, indicated temperature curve, heat release rate and the species at the end of combustion can be calculated. From these results, further engine characteristic results like combustion phasing, power output, torque output etc. can be calculated.

3.3. 1-D System Simulation

The 1-D system simulation simulates the entire engine system, including the auxiliary systems like the charging system, after-treatment, cooling, or pre-heating system, in the flow path dimension. The 1-D model is of high importance for developing the application engine and for optimize of the combustion system. The simulation was performed using Gamma Technologies GT Power. Most of the available predictive conventional combustion models in the software are empirical models, and no combustion model for validating the dual-fuel HCCI model was available. Hence, the kinetic-mechanism-based predictive combustion model should be used. The entire testbench system is modeled along with the conditioning and auxiliary systems, see Figure 2, and the pressure drop models will be validated based on experimental results. The heat transfer models are to be calibrated through setting model parameters, so that the simulated pressure curves and heat release curves correlate to the measured engine data. The effects of the heat of vaporization are also considered in this simulation through modelling of the fuel injection. Using this system model, the various auxiliary and control systems parameters, such as turbocharger sizing, cam phasing, injection phasing, pre-conditioning, etc. in the engine can be optimized.

3.4. 3-D CFD Simulation

In this work, a numerical model for an HCCI engine was developed using AVL FIRE M. The CFD model provides insight into the details of the physiochemical processes during intake, compression, atomization, ignition, combustion, and emission formation. From the 3-D CAD model of the combustion chamber and the port of the single-cylinder engine and some engine parameters, a dynamic mesh was created of the piston and valve movements. The unsteady Reynolds-averaged Navier-Stokes (URANS) simulation used the k-zeta-f turbulence model. The injection model is based on the Lagrangian approach and uses the discrete droplet model (DDM). The validation of the models to accurately represent the spray width and penetration was done with the help of optical measurements of the fuel injection. The model has a direct coupling of gas phases and chemical kinetics through the GGPR module, which provides source terms for species and enthalpy, that are considered in the conservation equations. This coupling enables to capture of the combustion characteristics of the engine.

The goal of the simulation is to gain a deeper understanding of the combustion processes and to optimize parameters including valve and injection timing, residual gas content, piston and injector design etc. The effects of local distributions of temperature and mixture composition in the cylinder on the combustion process and emission formation can be investigated. The interaction of turbulence and kinetics on the auto-ignition behavior is considered in the 3-D simulation. The influence of the combustion chamber geometry on the homogeneity and mixing behavior of the air and injected fuel can be investigated and the results can be used to improve the piston design and optimize the injector, and change the injection time.

4. Discussion and Future Work

An innovative combustion dual-fuel HCCI concept is being developed, where the RCCI combustion concept is modified by early injection of the high-reactivity fuel, and using only the overall mixture reactivity to phase the combustion. Using the aforementioned simulation methodology, the proposed dual-fuel HCCI model is simulated, and the pressure, temperature, and heat transfer results from test results can be used to calibrate the model parameters. These models will form the baseline for further simulations of the engine, optimization of various control parameters, including cam and injection phasing, pre-conditioning, turbo-sizing, etc., and design refinements of components, including the piston, intake port, and injectors. These optimizations are vital for achieving our aim to reduce the engine out emissions and to increase the overall efficiency.

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