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Direct numerical simulation of the effect of compression on the flow, temperature and composition under engine-like conditions

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Abstract

The effect of compression on the flow, temperature and composition inside a cylinder is investigated using direct numerical simulation (DNS). The initial conditions are obtained by a separate DNS of the intake stroke in an open-valve setup which includes thermal and species mixing. The results show significant changes of the turbulence and temperature fields during compression: The decrease of kinematic viscosity resulting from the increasing pressure results in smaller turbulent length scales and higher dissipation rates. Temperature fluctuations away from the walls decrease slightly during the first half but increase strongly during the second half of the compression stroke towards the Top Dead Center (TDC) due to heat transfer to and from the walls and turbulent transport. At TDC the turbulent flow field is anisotropic, and the axial fluctuation velocity is approximately 30% smaller than the fluctuation velocities in the radial and azimuthal directions. The integral length scale of temperature is approximately 25% higher than the integral length scale of turbulent kinetic energy. The stratification in the species concentration is found to be practically negligible.

Keywords: Direct numerical simulation; Internal combustion engine; HCCI; Compression; Thermal stratification

1. Introduction

Homogeneous charge-compression ignition (HCCI) engine concepts offer the potential of increased efficiencies with very low NO_x and soot emissions [1]. The higher efficiency can be achieved by higher compression ratios, absence of throttling losses and thermodynamically-favorable nearly-isochoric combustion [2]. However, the rapid heat release also results in increased stresses on the engine structure and noisy operation [3]. Reduced NO_x and soot emissions result from the relatively low peak combustion temperature attained by lean mixtures or high External Gas Recirculation (EGR) rates and well-mixed operation. In contrast to soot and NO_x, higher CO and unburnt hydrocarbon emissions are due

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to temperature and/or mixture inhomogeneities close to the cylinder walls [4]. Inhomogeneities have a strong influence on the temporal development of the heat release, since hotter and fuel rich regions tend to ignite before zones with less favorable ignition conditions. Temperature stratification has a strong influence on the autoignition behavior through the exponential dependence of the reaction rate on temperature, and can be beneficial for reducing the knocking tendency by lowering the rate or pressure rise.

Sjöberg et al. [5] assessed experimentally the effect of increased thermal stratification on HCCI combustion and found it to be beneficial in significantly extending the high-load operating point. Recently, several studies employed 2-D DNS to describe the influence of weakly thermally stratified initial conditions on the HCCI autoignition chemistry (e.g. [2,6–10]). In Ref. [2,6], the autoignition behavior was investigated for different artificial turbulent and temperature initial conditions of a homogeneous H_2/air mixture at 41 atm. The fluctuations of a zero-mean velocity and constant-mean temperature fields were initialized using a Passot–Pouquet spectrum [11], which requires the most energetic wavenumber and the fluctuation velocities as input parameters. Temperature fluctuations were found to have a strong effect on the combustion mode, the timing and the duration of the heat release rate leading to advanced ignition, longer combustion and to a significantly higher fuel consumption rate due to deflagration instead of homogeneous ignition.

Under real engine conditions, turbulent quantities like the integral length scales or fluctuation velocities are difficult to measure or estimate and are expected to vary significantly within the domain. Insight into the flow and temperature fields in engines before ignition can be obtained using high-speed Particle Image Velocimetry (PIV) and/or Laser-Induced Fluorescence (LIF) measurements. One of the first applications of 3D PIV measurements in engines [12] recently investigated the flow field in a cube of dimensions $47 \times 35 \times 4\ \mathrm{mm}^3$, with a spatial resolution of 0.4 mm in each direction. Recent LIF measurements are reported in Refs. [13–15]. In these works the temperature distributions were obtained on vertical slices with a spatial resolution of approximately 0.4 mm. In contrast to [13], the results of [14,15] showed increasing thermal stratification towards Top Dead Center (TDC). The PIV and LIF measurements were performed on planes or small volumes within the domain, which provide a valuable but limited insight on the flow and temperature fields inside the cylinder. In addition, measurements close to the walls are challenging and it is difficult to resolve the thin transient boundary layer which has a strong influence on the thermal stratification during compression.

DNS offers the advantage of high spatial and temporal resolution. However, due to the high computational cost, few simulations of complex geometries with moving boundaries can be found in the literature. Güntsch [16] studied the effect of compression on artificial turbulence in 3D cylindrical geometries with a compression ratio of 4.2. The effect of different piston speed profiles and the influence of swirl were investigated by statistical analysis (mean and fluctuating quantities, PDFs, two point correlations, turbulent length scales, statistical moments of third and fourth order and energy density spectra).

In Ref. [25], the incompressible flow and cyclic variability in the valve/piston assembly studied experimentally by Morse et al. [24] was investigated using DNS. Starting from the numerical data of the latter, a precursor simulation was performed to compute the mixing of a cold mixture with the hot gases inside the cylinder and obtain engine-relevant initial conditions for the work presented in this paper. Despite its simplicity, the setup considered here preserves many features of the dynamics of real engine flows (e.g. jet breakup during the intake stroke, interaction of the jet flow and shear layers with the walls and the remaining turbulence at TDC of the previous cycle). In addition, the axisymmetric geometry allows for spatial averaging, which heavily reduces the simulation time for comparisons with RANS or LES simulations. The relatively low engine speed of 560 rpm which is dictated by the computational cost is representative of idle conditions in a variety of ICEs.

The aim of this work is to obtain 3-D spatio-temporal data at a resolution that cannot be provided even by sophisticated experiments in the cylinder of a laboratory-scale setup and to study the effect of compression on the flow, temperature and species distributions.

2. Computational method

The low Mach number form of the conservation equation are integrated in time with a highly-efficient parallel code based on nek5000 [17]. The solution is expressed in terms of tensor products of nth-order Lagrange polynomials based on the Gauss–Lobbato–Legendre quadrature points [18] within hexahedral conforming elements. Time integration employs a high-order time splitting scheme for low Mach number reactive flows [19], whereby the continuity and momentum equations are integrated with a semi-implicit scheme and the species and energy equations are integrated implicitly using CVODE [20].

The Arbitrary Lagrangian/Eulerian (ALE) approach is employed to account for the mesh variation resulting from the piston movement. The ALE implementation described in Ref. [21]

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