SMARTCATs COST Action

Short Term Scientific Mission Report
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Details of STSM :

STSM title: Computational Fluid Dynamics (CFD) analysis of auto-ignition inside a Rapid Compression Machine using a detailed chemical kinetic mechanisms

Reference: COST-STSM-ECOST-STSM-CM1404-010916-079615

Period:2016-09-15 to 2016-12-15

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Introduction

The STSM program was perceived with Vrije Universiteit Brussels to gain expertise in the field of Computational Fluid Dynamics using detailed chemical kinetic models.

Rapid Compression Machines are the experimental facilities which are used for understanding the low to intermediate temperature auto-ignition chemistry under engine like conditions. RCMs are used to measure global parameters like ignition delay times as a function of temperature, pressure and fuel-air ratio. The high piston

velocities during compression raises complex fluid mechanics effects like roll-up of the boundary layer, bringing the cooler gases from the walls to the center of the chamber. This causes the temperature inhomogeneities which is major drawback for exact predicting of adiabatic core temperature. Therefore, an addition of a crevice on the piston can eliminate the complicate fluid mechanics and the unwanted mixing with the near-wall cold gases inside the combustion chamber, resulting in a homogeneous mixture[1][2].

Though, the creviced pistons shows significant advantages in predicting better temperature inside the core chamber. The temperature inhomogeneities inside the reaction chamber, due to wall heat transfer cannot be avoided. These induce spatial variations in terms of chemical composition, significantly affecting the autoignition process. The purpose of this STSM is to compute Computational Fluid Dynamics (CFD) simulations coupled with wall resolved RANS solver for the dimensions of the Rapid compression Machine used to perform experiments in PTB. This helps to characterize the state of reacting mixture and the causes of temperature inhomogeneities inside the reacting chamber.

Description of the numerical tools

The 0-D and RANS simulations are performed using open-source library OpenFOAM® [3]. The RANS simulations are performed by finite volume solver which, uses the PIMPLE algorithm which essentially combines the PISO (Pressure Implicit with Splitting of Operator) and the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithms. Convective terms of the density, momentum and species equations are discretized using a first-order upwind scheme while a centered scheme is used for other terms. The RANS equations are solved using the k-ω-SST turbulence model [4]. This model performs well in adapting the turbulent viscosity according to the flow topology, e.g. avoiding unreasonably high dissipation levels in the wall-region as the classic k-ε does. The fluid dynamics and chemistry interactions are simulated by TDAC (Tabulation of Dynamic Adaptive Chemistry) algorithm, which essentially couples the DAC (Dynamic Adaptive Chemistry) [5] and

the ISAT (In-Situ Adaptive Tabulation) [6] algorithms. This decreases the impact of number of species and of the number of the cells on the computational cost.

Zero-dimensional simulations

The zero-dimensional simulations are conducted by considering an homogeneous reactor model (HRM). A widely used approach, followed here, to account for heat losses during compression and post compression period is to apply the classic adiabatic core assumption together with a volume expansion term [7], while the loses during the compression are modeled by an additional volume V_{add} . The “effective volume approach “which is used to prevail the modeled temperature and pressure conditions similar to center of the reacting chamber. This approach can be explained by following equations [8]:

$$V_{eff}(t) = V(t) + V_{add} \qquad (t \leq t_{TDC})$$

$$V_{eff}(t) = V_{eff}(t_{TDC}) * f(t) \qquad (t > t_{TDC})$$

An empirically determined parameter, V_{add}, is added to the actual time-dependent geometric volume of the combustion chamber, V(t), to match the simulated pressure at the end of compression stroke, $t = t_{TDC}$, with the experimental P_C value. f(t) is a stretch function being commonly adjusted to fit the simulated non-reactive pressure trace to the experimental non-reactive pressure trace.

The 0-D simulations of RCM experiments are performed with OpenFOAM code. The experimental pressure traces are considered from Mittal et.al experiments [9] of using a mixture H2/N2/Ar of the same specific heat, initial temperature, initial pressure of reactive mixture. Fig 1. Shows a comparison for experimental non-reactive pressure trace of P_0 = 705.8 Torr and T_0 = 298 K. The simulated pressure trace are obtained from considering hydrogen and syngas mechanism of A.keromnes et.al [10]. The aforementioned conditions are considered to valid the 0-D modelling.

Similarly, a refinement of ammonia combustion model is to done by considering the experimental data of ignition delay of pressure (20-60 atm) and temperatures of (700-1100 K) with equivalence ratios 0.5, 1.0, 2.0. Furthermore, the RCM trajectory is to analytically deduced from the geometrical properties of the machine. This is taken as input as the piston starts from rest and move same as of real RCM. This work is in underway and will be completed as soon as possible to analyze the inhomogeneities inside the RCM.

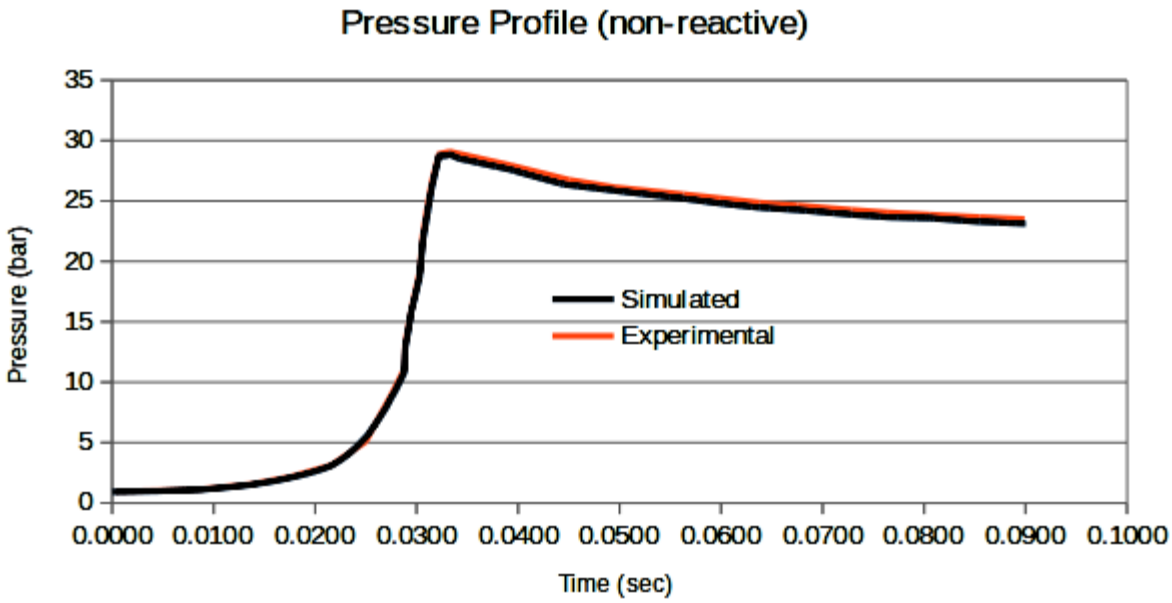

Fig 1. Comparison of experimental and simulated pressure traces of H2/N2/Ar mixture of P_0 = 705.8 Torr and T_0 = 298 K.

Numerical Study

The numerical study was carried out in two steps. First, the geometric specifications of the creviced piston of PTB rapid compression machine is considered. The computational domain is discretized using hexahedra meshing. Second, the discretized computational domain is considered to simulate 2D RANS calculations.

A wall type of boundary condition is considered at the top boundary, which classically correspond to cylinder head. This is due to single piston RCM. An illustration of the mesh at TDC is shown in fig 2. The mesh near to wall is resolved to ~ 10 μm due to the respect of $y^+ < 1$ constraint and spatial variations are located close to the

walls. The coarse mesh away from walls is due to high level homogeneity inside the reactive chamber and this does not require to refine mesh away from walls.

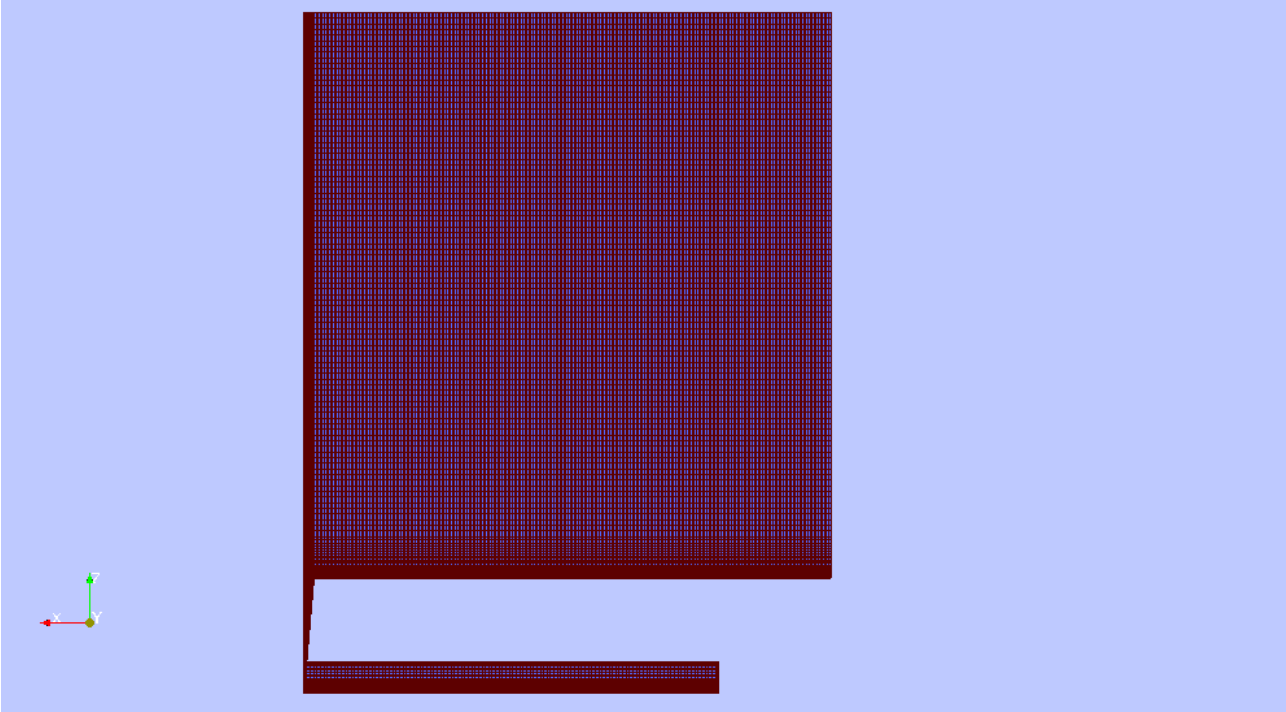

Fig 2. Illustration of wall resolved mesh at TDC. The piston moves in z-direction.

RANS Simulations

The results of RANS simulations are still being processed.

Future collaboration with host institution

Given the extensive experience of the CFD modeling research group in modeling reacting flows of Vrije universiteit Brussels, and the wide experience of the combustion research group of PTB, Braunschweig in experimental work, I believe there is a high potential for further collaboration in the future.

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