A numerical study, implementing chemical kinetics, to assess pre- and post-spark self-ignition in a hydrogen internal combustion engine

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Abstract

The onset of possible undesired events such as pre-ignition and end-gas autoignition that may or may not lead to knock in a spark ignition hydrogen ICE is investigated through a 3D CFD analysis implementing gas phase reactions. The chemical kinetic mechanism by Keromnes-2013 has been chosen for this objective based on its performance against different other mechanisms available in the literature providing the least discrepancy for ignition delay times against Shock-Tube and Rapid-Compression-Machine experiments. A typical commercial vehicle engine with an internal single displacement of about 2l equipped for a Direct Injection SI-H_2 engine has been used, for which experimental test bench data are available to be compared against the numerically reproduced engine cycle. The spatial and temporal distribution of the reactive intermediate species, temperature, pressure, and equivalence ratio have been thoroughly investigated in a commercial CFD code AVL Fire Classic. Regions of mass and thermal inhomogeneities particularly around the spark plug, valves and the injector were monitored for which the charge mixture could possibly evolve into an abnormal combustion depending on the local thermodynamic state being close the explosion limit of the H_2-air mixture at that localized equivalence ratio. The results of the current fundamental but essential analysis could become an objective function for H_2-ICEs to design optimal charge-motion and cooling techniques minimizing mass and thermal inhomogeneities respectively of a H_2-air mixture inside the combustion chamber to ensure a safe engine operation.

Introduction

The goals set by the EU green deal [1] to achieve zero-carbon emissions have led the automotive sector towards focused research on Hydrogen Internal Combustion Engines (HICEs) among many other hybrid and electric propulsion alternatives. Hydrogen, with its intrinsic characteristic to be burnt lean due to its wide

flammability range, and just with water as the main emission, if the considered mixture is pure H_2-O_2, is a viable and attractive solution to achieve the zero-carbon emissions target. While trying to maintain the balance between performance and selection of geometry for a HICE [2], the industry's objective to acquire the correct design parameters has mainly been limited by the occurrence of pre-ignition [3–5]. In Direct Injection (DI) engines, such as the one of the present study, pre-ignitions could be caused by thermal and mass inhomogeneities around the injected hydrogen jet. The mass inhomogeneity allows different fuel-air equivalence ratios around the injection where a richer mass fraction of the mixture may pre-ignite the charge. Thermal inhomogeneities promote temperature gradients within the mixture around hot-spots such as high temperature exhaust deposits and spark plug tips. The formation of hot-spots, such as soot particles and deposits on spark plugs, is caused by the pyrolysis of lubricating oil [6–8]. One of the major reasons of pre-ignition in HICEs is through contamination of the pure H_2-air charge with lubricating oil. This contamination alters the mixture composition and therefore its chemical state promoting a much earlier ignition. The presence of lubricating oil in the primary charge and its role in pre-ignition phenomenon has been recently investigated by Distaso et al. for the case of hydrogen [9,10].

Considering SI engines, engine knock or detonation can be caused by the interaction between the propagating flame front and the detonation wave [11,12] generated at a hot-spot within the end-gas. To understand the possibility of such an event, it is crucial to know the chemical and thermodynamic state of the end-gas which may or may not ignite due to that hot-spot. In essence, pre-ignition of hydrogen fueled engines can be explained by the hydrogen-oxygen chain reaction [13].

The onset of a self-ignition event can be explained through the assessment of explosion limits of the H_2-air mixture. The explosion limit of a fuel-oxidant mixture is the locus of pressure and temperature values that distinguish between an explosive and non-explosive reaction of the said mixture composition. This limit, in practice, is an isometric line with a constant value of ignition delay time and has been first reported experimentally by B. Lewis and G. von Elbe [14] for H_2-O_2 mixture at stochiometric conditions acquired in a constant-volume spherical chamber.

Whether the occurring abnormal combustion event is either pre or post ignition, both scenarios cause peak pressures beyond a safe limit that damage the engine components. These limits are typically recognized through engine test bench experiments by performing a Design of Experiments (DOEs) with variable parameters like intake pressure, temperature, and mixture composition. These exhaustive experiments, however, can be reduced by having at hand a numerical and systematic method for analyzing and consequently preventing adverse combustion effects like pre-ignition or end-gas autoignition. The use of numerical chemical kinetics allows for such possibility to evaluate in-cylinder thermodynamic states that could promote an undesired combustion during engine operation. To expand this numerical study in 3D, the current CFD study, implementing gas-phase reactions, is performed.

Methodology and simulation setup

To assess the possible transition of any local thermodynamic state towards an abnormal combustion event either before the initiation of the spark (pre-ignition) or after the spark has been initiated (i.e., post-spark-ignition e.g., end-gas auto-ignition) inside the combustion chamber, it needs to be compared with the explosion limit of the charge mixture. This requires having the in-cylinder spatial and temporal distribution of pressure "p", temperature "T", and mixture composition (equivalence ratio "ϕ") through a 3D CFD analysis. The explosion limit for H_2-air mixture can be acquired numerically through a 0D homogenous batch-reactor simulations for a range of p, T, and ϕ values. Such simulations have been performed on Ansys CHEMKIN Pro software utilizing the Kéromnès mechanism [15] to acquire explosion limits having isometric ignition delay times of 1ms. At current engine speed i.e., 1300 rpm, one stroke is completed in about 23 ms, so selecting 1ms as threshold is most appropriate for engine applications.

For the numerical analysis a typical commercial vehicle engine with an internal single displacement of about 2l has been used. CFD mesh details and numerical setup are reported in **Table 1**. Valve close injection and combustion events, and their corresponding Crank Angle Degrees (CADs) are listed in **Table 2**. A full engine cycle has been simulated in a commercial CFD code AVL Fire Classic implementing boundary and initial conditions at each stage acquired from the test bench experimental data for the operating point in question. The thermodynamic states of pressure, temperature for relevant intake conditions and injection parameters are reported in **Table 3**.

Table 1 Mesh parameters & numerical setup

Mesh cell shape	Hexagonal
Solver	unsteady RANS
Turbulence model	k-ζ-f

Table 2 Valve, injection and spark timings.

End of compression stroke	Simulation start point	0° (Top Dead Center)
Start of Injection	SOI	597°
End of Injection	EOI	650°
Spark timing	ST	704.9°

Table 3 Thermodynamic states at intake valve opening and injection parameters.

Pressure at IVO	p_{IVO}	2.918 bar
Temperature at IVO	T_{IVO}	45.4°C
Equivalence ratio at EOI	ϕ_{EOI}	2.4
Injection pressure at SOI	p_{inj}	23.678 bar

Results

After the validation of the numerical pressure trace with experimental, cross-sectional plots for p, T and ϕ were created to analyze the spatial distribution of each parameter.

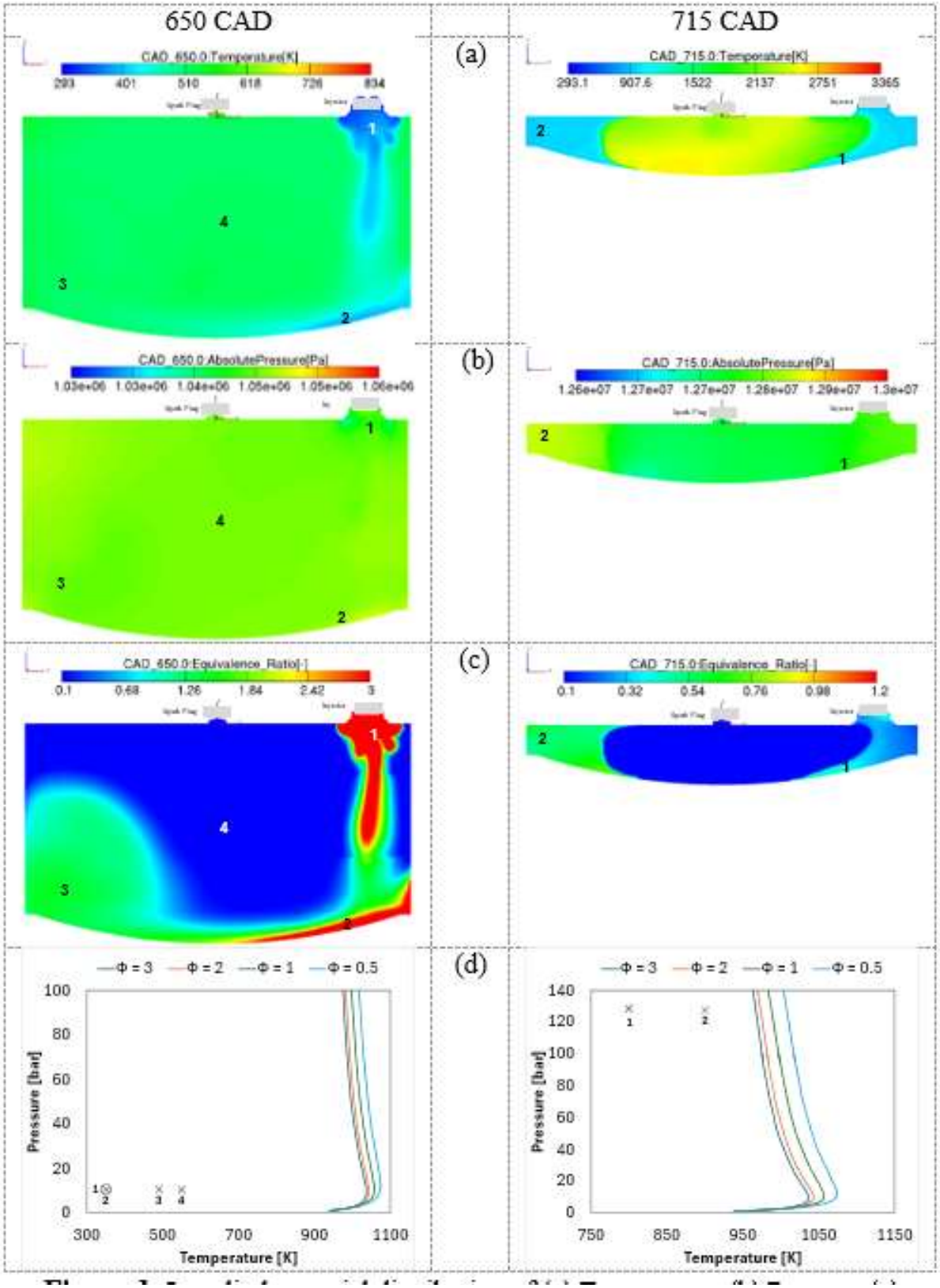

Figure 1 represents two different time instants inside the cylinder, namely, 650 CAD (EOI) and 715 CAD (~13CAD after the ST) to compare any local thermodynamic state that could reach or even surpass the explosion limit. Within the figure the spatial distributions of p, T, and ϕ (

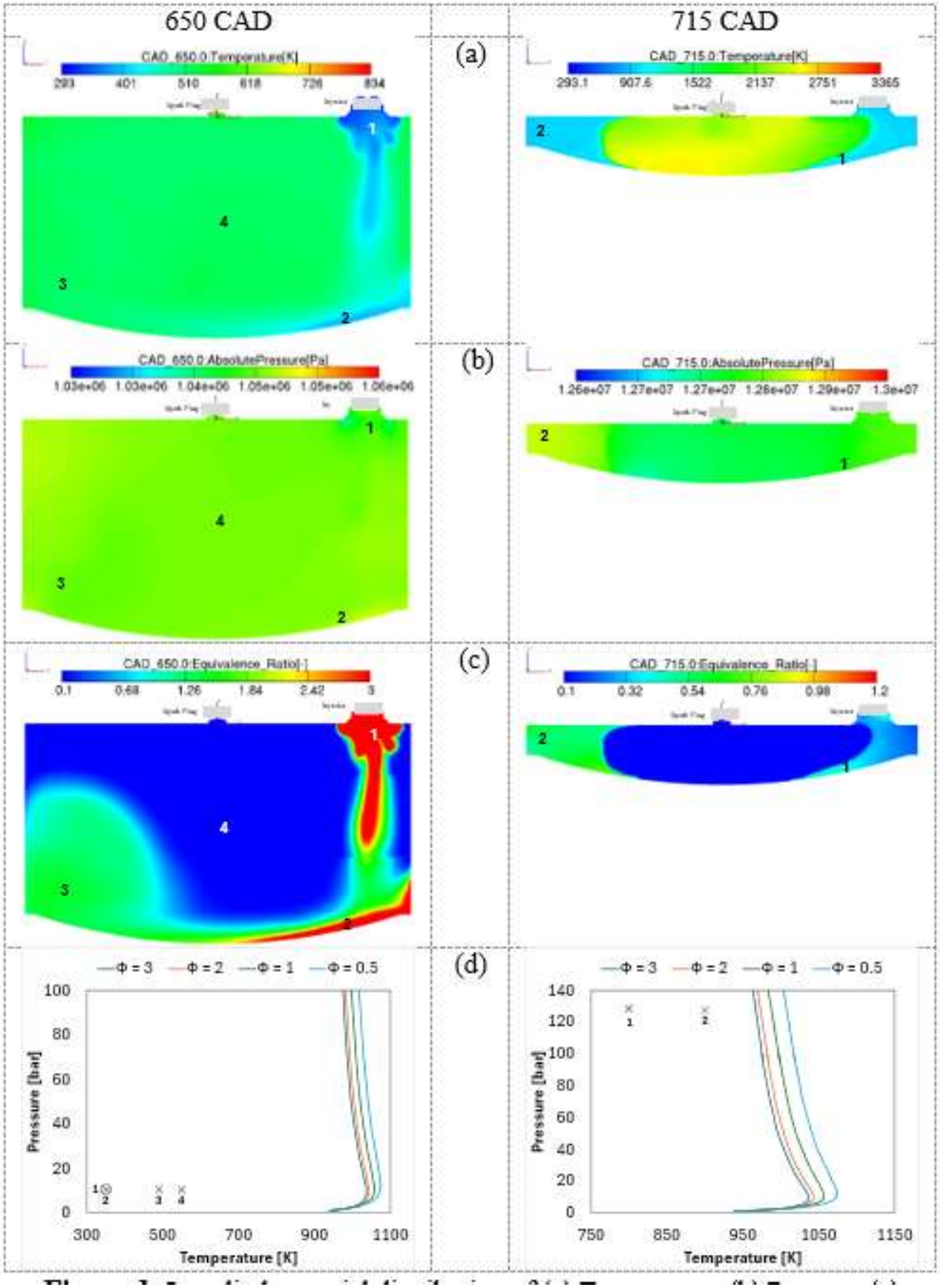

Figure 1(a)(b)(c)) are shown. Knowing these three variables allows one to plot the same on a p-T plot (

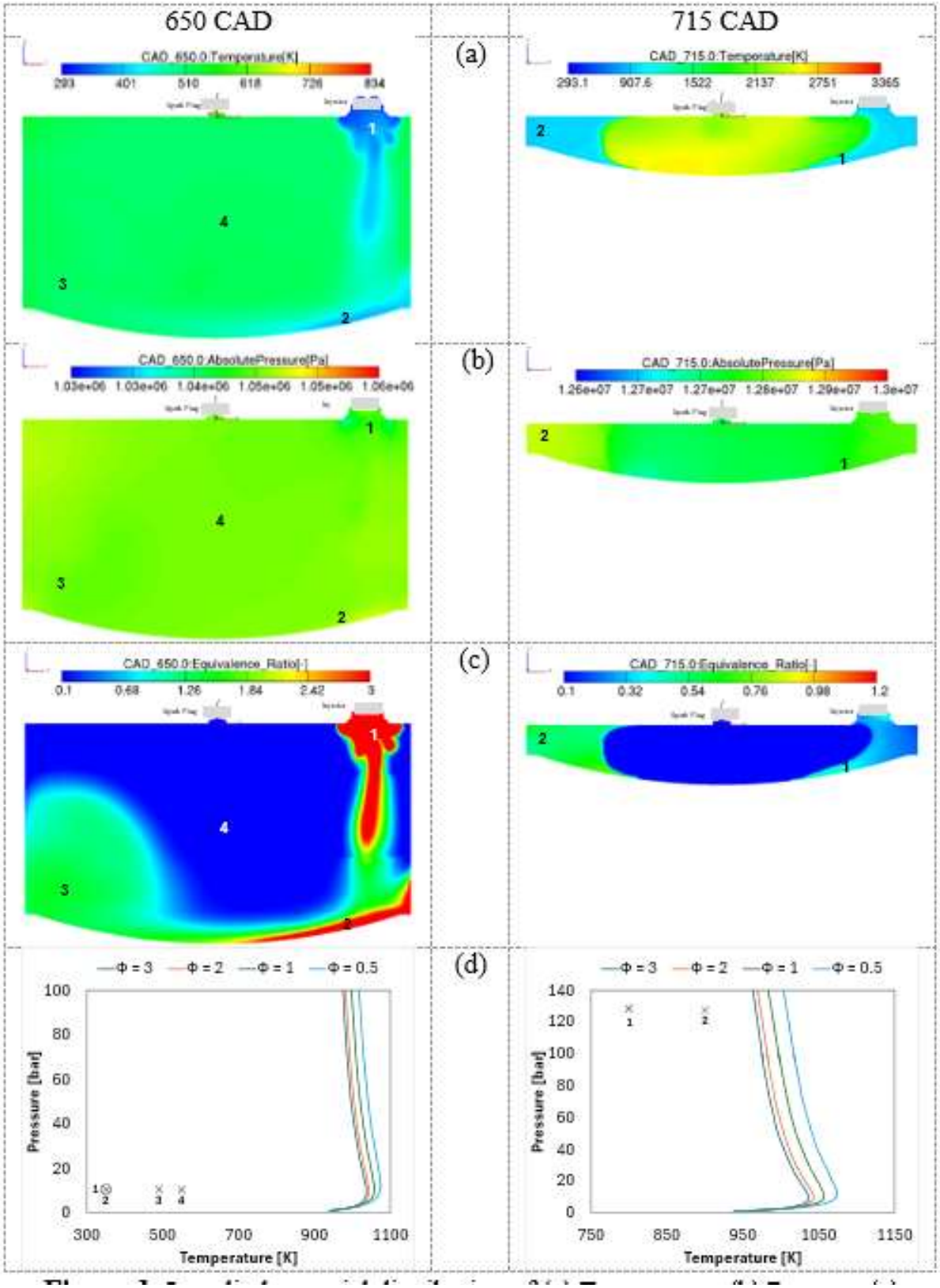

Figure 1(d)) and compare the state against the explosion limit. A few in-cylinder points, chosen for each time instant (mentioned on each plot), are considered for comparison on the p-T plot.

It is observed that for 650 CAD (EOI), none of the four thermodynamic points

reaches conditions close to the explosion limit even at the higher end of $\phi = 3$. Despite the high equivalence ratio close to the injector, both the localized pressure and temperature are not enough to bring the thermodynamic state close to the explosion limit. The cooling effect can also be observed because of hydrogen jet expansion upstream the injector.
For the second case (715 CAD), point 2 gets in the vicinity of the explosion limit at $\phi = 3$ but not close to that of $\phi = 0.5$ to which it corresponds. Even though point 2 is away from evolving into an abnormal combustion event, it clearly shows its higher thermodynamic state as the compression wave generated by the moving flame front compresses the local mass of charge close to the walls [16]. A higher rate of combustion or higher intake conditions at IVO could possibly induce such an undesired combustion.

Conclusions

The present CFD study paves the way towards development of an integrated database for H2 combustion, which would be an invaluable resource for designing H2 engines in a safe manner, avoiding undesired pre- and post-spark self-ignition during engine operation. This fundamental study evaluates the thermodynamic states both spatially and instantaneously while monitoring their vicinity to the explosion limit. Further studies in the future will entail understanding an accumulation of heat release within the gas-phase reactions as well as imposing hot-spots at expected surfaces like valves and spark plug that could, in general, emulate an engine operating under real conditions.

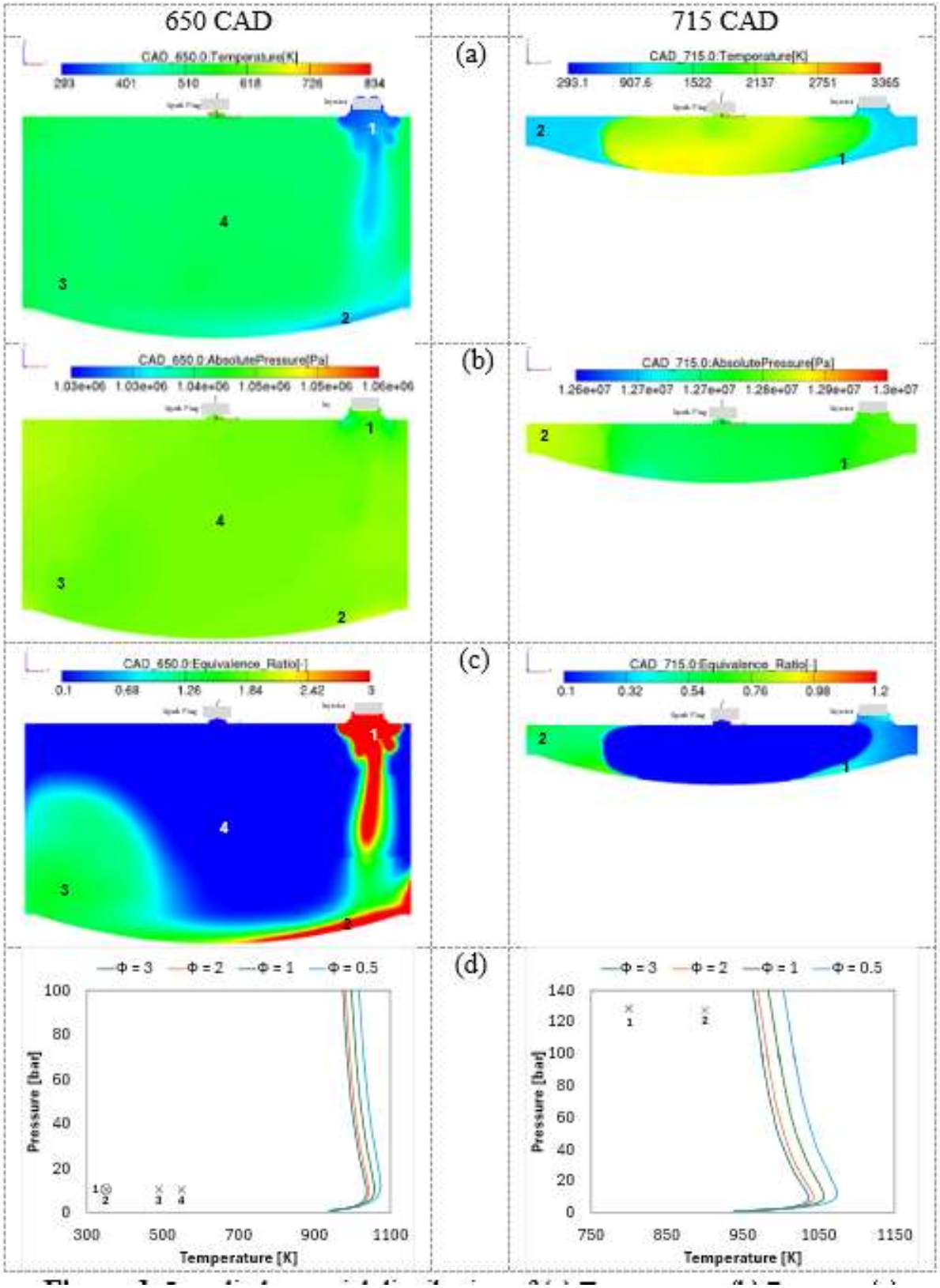

Figure 1. In-cylinder spatial distribution of (a) Temperature (b) Pressure (c) equivalence ratio, and (d) 1ms isometric explosion limits for varying phi values.

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