Self-ignition scenarios after rapid compression of a turbulent mixture weakly-stratified in temperature

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Abstract

Turbulence and combustion inside a compression machine, experimentally studied by Guibert et al. [Flow Turbulence and Combust. 84 (1): 79–85, 2010], are simulated to get some insight on flow-physics and ignition scenarios of a reactive-gas mixture pushed by a piston through a turbulence-grid, to be compressed in a 55 cubic-centimeter volume. Large Eddy Simulation (LES) with a structured-mesh solver and immersed boundaries are first performed for an inert mixture undergoing the compression, to validate the simulation procedure against experimental results. Then, keeping the flow admission-sequence the same, but downsizing its geometry, a Direct Numerical Simulation (DNS) analysis of the compression/ignition sequence is reported. Simulation parameters are varied for ignition to occur in mixtures featuring various temperature stratification patterns, due to wall cooling and turbulence characteristics. As previously discussed in the literature, conditions favoring spotty- or homogeneous-ignition are evidenced. Depending on characteristic times (coherent structure residence time, flow engulfment and mixing times) ignition may occur within localized compression zones, between vortical structures leading to spotty-ignition, or more homogeneously within large scale flow structures. Very small differences in local temperature and flow topology appear to lead to different routes toward successful auto-ignition. The underlying mechanisms are analyzed from an internal energy budget expressed as a temperature balance equation, to delineate between the contribution of the global adiabatic compression and localized flow divergence induced by turbulence velocity fluctuations. After primary ignition, the propagation phase of ignition is strongly influenced by the acoustic field and the specific temperature scalar dissipation-rate patterns. It is also shown that three-dimensional vortex stretching plays a crucial role, hence two and three-dimensional DNS lead to different ignition scenarios under similar chemical and turbulence intensity conditions.

1. Introduction

Even in the case of an injected charge featuring a perfectly homogeneous fuel/air equivalence ratio, inhomogeneities always exist in engine cylinders, as for instance temperature fluctuations because of wall cooling. These fluctuations add to the temperature rise due to the global compression and depend on the overall and local flow properties. During and right after the rapid compression, the flow is stratified in temperature, with an almost adiabatic core surrounded by zones of lower temperature, where heat diffuses toward cylinder walls. The primary ignition sites will thus be influenced by small differences in gaseous mixture internal energy, controlled by the specific flow topology and device geometry.

The physics of ignition at constant pressure or constant volume has been the subject of multiple studies, see [1–7] and references therein, some of them examining specifically ignition in the presence of vortical structures [8–12], mostly at constant pressure. Among the numerous results reported, two main ignition scenarios were discussed delineating between almost homogeneous- and fragmented- (spotty-) ignition regimes.

Recently, numerical simulations of laboratory engines have made great progress addressing cycle-to-cycle variations and other concerns with Large Eddy Simulation (LES) [13]. Detailed combustion chemistry plays here a major role and Direct Numerical Simulation (DNS) including a refined description of chemistry was also used for understanding the influence of chemical paths on ignition, in the case of non-uniform temperature and at constant volume for two-dimensional flows [14].

The flow topology is known to have a tremendous impact on ignition, also the objective of the present work is to analyze ignition scenarios in a context as close as possible to an existing experimental system. LES of engine combustion-chambers would lack of resolution to identify the detail of ignition processes. DNS with detailed chemistry is either two-dimensional or in canonical geometries for resolution constrains, thereby not including the key
features of real flow dynamics, which are responsible for temperature fluctuations appearing within wall boundary layers, along with the complex and specific flow patterns resulting from admission and subsequent rapid compression. A complementary route is attempted in the present study; the geometry of a rapid compression machine experimentally investigated by Guibert et al. [15–17] is considered at first with LES, to calibrate a three-dimensional simulation procedure with an admission sequence into a cylindrical combustion chamber through a turbulence-grid. Then, keeping the same flow admission velocity sequence, the system is downsized for DNS, with a resolution of about 20 μm. The overall simulation procedure can be compared with experiments and the flow and temperature distributions observed in the DNS are not arbitrary, but result from the experimentally observed admission–compression sequence. However, because of resolution requirements, simple chemistry is used, therefore only the interaction between a generic heat-release ignition process and the turbulent flow is reproduced, where phenomena induced by multiple chemical time scales are overlooked. (At the pressure at which ignition occurs in the machine, any chemical mechanism involving intermediate species would require a mesh much thinner than 20 μm.)

During admission in the combustion chamber considered, large-scale vortices are generated along with grid turbulence fluctuations. While the temperature rises because of compression, temperature fluctuations also develop with heat transfer at wall and temperature gradients are expected mainly in the flow zones close to wall and bordering large-scale coherent vortices, where fluids of different temperature mix. These large-scale flow rollers have a given residence (or life) time and the temperature distribution in their core evolves according to three mechanisms: adiabatic compression that goes with a uniform increase of temperature, engulfment of surrounding fluid and molecular diffusion, which promotes a local temperature stratification. Each of these mechanisms has a characteristic time scale; for instance if compression is rapid enough, a range of time exists over which core volumes of gas are mainly affected by adiabatic compression, therefore with a continuous increase of temperature, before much more complex flow temperature distributions appear, because of turbulent mixing with colder wall-layer fluid. In terms of phenomena controlling ignition, a competition between an almost adiabatic compression and turbulence properties driving fluid engulfment and mixing with colder mixture may thus be expected.

The numerical procedure and the geometry of the rapid compression machine are presented in the next section with LES results. Then, analyses of three-dimensional DNS are performed, the flow and temperature properties at admission are first examined, before looking at the ignition phase. To compare with three-dimensional flows and isolate phenomena, additional two-dimensional simulations are performed, before drawing ignition scenarios and quantifying the departure from behavior pertaining to perfectly stirred reactors at constant pressure.

2. Numerics and rapid compression machine modeling

The geometry studied refers to the rapid compression machine reported in [15] and operating with a compression ratio of 15.6. This machine is mainly composed of an hydraulic system, a piston moving inside a pre-compression volume and the combustion chamber. Initially, at \( t = 0 \), the mixture to be analyzed is contained within a volume decomposed into the pre-compression chamber, a convergent section, the piston nose lodging section and the combustion chamber. The pre-combustion chamber is a 200 mm long stainless steel tube of 91.5 mm diameter through which the piston moves to rapidly compress the mixture. The convergent section is 50 mm long and connect the 91.5 mm diameter tube with the 40 mm diameter combustion chamber, that is 44 mm long. The end of the convergent section stops the piston, the whole volume of gas is thus compressed into the combustion chamber, with a known dead-flow volume trapped between the piston and the convergent (i.e. this volume \( V^{\text{dead}} \) of gas does not enter the combustion chamber). Figure 1 is a sketch of this device, including the notations used to parameterize the simulations. The combustion chamber is made of quartz, to provide optical access, and a turbulence grid is placed at its inlet, a more complete description of the experimental device may be found in [16].

The Navier–Stokes equations are solved in their fully compressible form with the structured-grid solver SiTCom (Simulating Turbulent Combustion) [18–20]. The convective terms are computed resorting to a fourth-order centered skew-symmetric-like scheme [21], while the diffusive terms are discretized with a fourth-order centered scheme. Time is advanced with a third-order Runge-Kutta method [22] and the boundary conditions are prescribed with 3D-NSCBC [23,24]. The inlet-plane temperature follows an increase due to isentropic compression; in the boundary conditions, a strong relaxation towards this time evolving target value is imposed in 3D-NSCBC. To simulate a cylindrical combustion chamber over a cartesian grid, immersed boundaries are used with a ghost-cell approach to impose wall conditions inside the mesh, with bi- and tri-linear interpolations [25–27]. A Neumann condition is imposed for \( P \), the pressure, \((\partial P/\partial n = 0 \), where \( n \) is the direction normal to the immersed surface) and Dirichlet conditions are used for the no-slip velocities. According to experimentalists, moderate heat transfer occurs at the combustion chamber wall, this transfer has a weak impact on the thermodynamical compression properties, but influences the detail of the local temperature distribution within the chamber; the heat exchange at the wall temperature is computed with a temperature convection coefficient fixed at 40 W m\(^{-2}\) K\(^{-1}\) to match experimental results. Then at the ignition time, the maximum level of temperature fluctuations is of the order of 50 K.

In the LES cases, the transport of momentum and mass by unresolved fluctuations is expressed with the Wall Adapting Local Eddy-viscosity (WALE) closure [28], which has been specifically designed to reproduce correct scaling at wall boundaries.

The only combustion chamber is simulated, at inlet the flow velocity is imposed during the 29 ms duration of admission in this chamber. To do so, both the time evolution of the bulk velocity and fluctuations must be prescribed, the former is calculated from the experimental measurement of the piston speed and the latter is approximated from properties of the turbulence-grid used. The expression in cylindrical coordinates of \( U(r, \theta, t) \), the streamwise velocity distribution, is given by:

\[
U(r, \theta, t) = U_{0}(t)F^{\circ}(r) + U(r, \theta, t),
\]

where \( F^{\circ}(r) \) is the direction normal to the immersion plane and \( U_{0}(t) \) is the velocity distribution, is given by:

\[
U_{0}(t) = \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial}{\partial r} \right) + \nabla \cdot \mathbf{u} + \frac{\partial}{\partial t} \mathbf{u},
\]

where \( \mathbf{u} \) is the incompressible velocity field.

Fig. 1. Diagram of the rapid compression machine [15]. \( D_{cc} \), \( V_{cc} \): Diameter and volume of the combustion chamber. \( V^{\text{dead}} \): Dead-flow volume. \( D_{pc} \): Piston diameter. \( x_{p}(t) \): Piston position. \( V_{pc}(t) \): Volume to be swept by the piston. \( x^{\circ} = x_{p}(t = t_{\text{precc}}) \): Top-dead-center position.
with \( U_o(t) \) the bulk flow velocity at inlet and \( F^*(r) = F(r)/F_o \) with \( F(r) \) a radial distribution and \( F_o = 2\pi R^2 \rho_{in} u_{rms}/2 \) an integral length scale \( \ell_i = D_{cc}/10 = 4 \ mm \), where \( D_{cc} \) is the diameter of the combustion chamber, and velocity fluctuations amplitude of \( U_o(t)/10 \), leading to a maximum turbulent Reynolds number of the order of 1200 and a Kolmogorov scale of the order of 20 \( \mu \)m. These parameters have been adjusted to best reproduce the experimental pressure signal downstream of the turbulence grid of 69 holes (3 mm in diameter). It is shown in Appendix A that the bulk velocity may be approximated from the experimentally measured piston position \( x_p(t) \) and piston speed \( x_v(t) \), shown in Fig. 2:

\[
U_o(t) = \frac{R_o}{1 + \frac{D_o}{R_o}} \left( \frac{D_o}{D_{cc}} \right)^2 x_v(t)
\]

with \( R_o = R_{cc}/\left( \left( \frac{\pi D_o^2}{4} \right) \left( x^0 - x_v(t) \right)/4 + V^0 \right) \), where quantities are defined in Fig. 1. Overall, this distribution controls the pressure time increase within the chamber. \( F(r) \), the radial velocity distribution also plays a major role, various shapes have been tested by comparing the simulated flow properties after compression against experiments. Among clues to build this profile, large scale jet Kelvin–Helmholtz instabilities are not observed in measurements in the vicinity of the admission plane, thus ruling out profiles featuring inflection point according to the Rayleigh criterion. The retained profile reads:

\[
F(r) = \max\left[ 0.5(\tanh(f_3 (f_2 - r/D_{cc})) + 1) - f_3, 0 \right]
\]

with \( f_3 = 9.000, f_2 = 0.355 \) and \( f_3 = 0.190 \).

LES performed to calibrate the simulations are all 3D, then the mechanisms driving ignition are first observed from three-dimensional DNS, to be studied also in a sequence of two-dimensional simulations for comparison. The LES grid is composed of 4,000,000 nodes with a characteristic implicit filter size \( \Delta = 0.24 \ mm \), therefore at inlet \( \ell_i/\Delta \approx 16.60 \). Once the simulation procedure evaluated, the volume is downsized by a factor 64 (resp. 16) for three- (resp. two-) dimensional DNS (i.e. each length is divided by 4), preserving the pressure signal of Fig. 3. The calculations are performed with 70,136,136 (resp. 272,420) grid points in 3D (resp. 2D), with a resolution of about 20 \( \mu \)m; 4096 (resp. 512) processors of an IBM Blue Gene/P machine are used.

The main interest in performing DNS within the framework of a real compression machine lies in the possibility of having both compression and velocity field as close as possible to those observed in experiments, even though, because of turbulence variability and resolution requirements, a fully exact numerical representation of such device is out of reach.

![Fig. 2. Measured time evolution of the piston speed, \( x_v(t) \) [15,16]].](image)

![Fig. 3. Reynolds average pressure vs time. Circle: experiment. Cross: LES.](image)

Figure 3 shows the time evolution of mean pressure in the chamber without combustion, for a mixture composed of \( \text{CO}_2 \) and \( \text{N}_2 \) with molar fractions \( X_{\text{CO}_2} = 0.65 \) and \( X_{\text{N}_2} = 0.35 \). The duration of admission is \( t_{\text{TDC}} = 29 \) ms, where ‘TDC’ denotes the top-dead-center. In the simulation, this compression is mainly controlled by Eq. (1), defining the time distribution of bulk velocity during admission, which allows for reproducing the experimental pressure signal (Fig. 3). Notice that without accounting for the exact piston speed (Fig. 2) and various flow volumes through the geometrical parameter \( R_o \), it was not found possible to simulate the proper pressure response.

Two-dimensional Particle Image Velocimetry (PIV) provided instantaneous snapshot of the velocity magnitude [15] to compare with three-dimensional simulations. Velocity from LES are filtered in space with a resolution that differs from PIV and thus cannot exactly match the measured one. Nevertheless, the major features of the strongly unsteady flow are captured, as seen in Fig. 4 displaying the velocity amplitude for three instants in time starting from top-dead-center. The rapid flow admission in the chamber first creates a centerline flow (Fig. 4a) that impacts the opposite wall to then fill out the chamber with decaying turbulence.

The average level of velocity fluctuations rapidly decays after top-dead-center (i.e. \( t > t_{\text{TDC}} = 29 \) ms in Fig. 5). To measure the turbulent kinetic energy, \( \langle K \rangle = 0.5(\langle u^2 \rangle - \langle u \rangle^2) \), PIV was performed over four instants in time and repeated for ten runs of the compression machine, the corresponding Reynolds averaged turbulent kinetic energy was estimated cumulating for every instant the 10 measurements. In LES, statistics are computed making use of the axisymmetric character of the flow: averages are first cumulated over the azimuthal direction, resulting in a single mean half-plane over which an average value is built. LES is sufficiently resolved for the molecular viscosity of the mixture to play a non-negligible role in the primary shear layers development, in the peak turbulence level and therefore in the first stage of the turbulence decay. As displayed in Fig. 5, only the \( \text{CO}_2/\text{N}_2 \) mixture with the Wilke law [30] for estimating the viscosity reproduces values close to experiment for \( t < 35 \) ms; here also it must be kept in mind that PIV and LES are not with the same filtered size and that the SGS part is not included in this comparison, but overall, results stay close to experiments, with a residual turbulence level higher in the experiments than in LES. In the following, ignition will be studied well before reaching \( t = 45 \) ms, therefore in the time range where simulation results stay close to measurements.

In the DNS reported below, chemistry is simplified to single-step under the hypothesis of fuel-lean combustion (e.g. there is an excess of air so that combustion weakly modifies oxidizer concentration) and unity Lewis number is assumed; the progress variable \( c = 1 - Y_f/Y_{f,o} \) (with \( Y_f \) the fuel mass fraction and \( Y_{f,o} \) its value.
This oversimplified description of chemistry allows for reproducing global properties of ignition following rapid compression along with the intricate coupling with turbulence and heat release; however, using a single time-scale for chemistry is a strong limitation of this study that must be kept in mind. For instance, any cool-flame effects that could be observed with heavy hydrocarbon fuels cannot be present; hence, when comparing with experiments, only the very first ignition can be studied, not the eventual temperature plateau and subsequent thermal runaway observed with heavy hydrocarbon.

3. Three-dimensional DNS analysis of auto-ignition in temperature-stratified mixture

3.1. Flow and temperature at admission

The birth of ignition in the rapid compression machine strongly depends on temperature rise, resulting from adiabatic compression interacting with wall heat-transfer. Part of the analysis of simulations may thus be conducted from the temperature balance equation [31,32]:

\[
\rho C_p \frac{DT}{Dt} = \nabla \cdot (\lambda \nabla T) + \dot{\omega}_T + \frac{DP}{Dt} + \dot{S}_v.
\]

(4)

Where usual notations are adopted, \( \rho \) is the density, \( C_p \) is the constant pressure heat capacity, \( \lambda \) is the heat diffusion coefficient and \( \dot{S}_v = T_0 (\partial u_i / \partial x_i) \) is the viscous dissipation, with \( T_0 \) the viscous tensor. \( D \psi /Dt = \partial \psi /\partial t + \mathbf{u} \cdot \nabla \psi \) denotes the Lagrangian derivative with \( \mathbf{u} \) the velocity vector. From continuity equation and perfect gas law \( P = \rho r T \),

\[
- \frac{1}{\rho} \frac{DP}{Dt} = \nabla \cdot \mathbf{u} = \frac{1}{T} \frac{DT}{Dt} - \frac{1}{T} \frac{DP}{Dt} + \frac{1}{T} \frac{Dr}{Dt},
\]

(5)

with \( r = C_p (\gamma - 1)/\gamma \) and \( \gamma = C_p/C_v \) with \( C_v \) the constant volume heat capacity. Relation (5) combined with Eq. (4) assuming constant heat capacities, lead to:

\[
\frac{DT}{Dt} = \frac{T}{P} \frac{DP}{Dt} + \nabla \cdot \mathbf{u},
\]

(6)

\[
= \frac{1}{\rho C_v} \left( \nabla \cdot (\lambda \nabla T) + \dot{\omega}_T + \frac{1}{\gamma - 1} \dot{S}_v \right) - (\gamma - 1) \nabla \cdot \mathbf{u}.
\]

(7)

The non-isentropic term \( \dot{S}_v \) is found small in the DNS database, with a negligible contribution to ignition (i.e. it is at least three orders of magnitude smaller than other terms of Eq. (7)).

During compression and before ignition, the Lagrangian temperature rise \( (DT/Dr) \) is driven by an adiabatic-increase part, due to the gas volumetric reduction, to which local variations are added because of heat-transfer at wall and local flow inhomogeneities. This is well summarized in Eq. (7), where three main terms are identified: (i) diffusive flux, (ii) chemical source and (iii) local flow divergence. In the form of temperature equation retained in Eq. (7), this term (iii) represents the temperature modifications due to the total contribution of \( \nabla \cdot \mathbf{u} \), which is a source when \( \nabla \cdot \mathbf{u} < 0 \). Before ignition, the term (ii) is negligible, however in the rapidly compressed mixture, a small temperature rise is sufficient to promote ignition starting (non-zero \( \dot{\omega}_T \)); the specific flow points where ignition will first start therefore depend on the behavior of temperature diffusion (term (i)) and local flow divergence (term (iii)), locally bringing temperature up to the required level for ignition to begin. Depending on the characteristic scales of turbulence and temperature fluctuations, ignition may thus be expected to develop differently.

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1. In the simulations, the energy equation is solved in its complete form, the simplified temperature Eq. (7) is introduced only for post-processing purposes.
Figure 6 shows turbulent structures colored by temperature in case (2), before ignition (because of identical turbulence level, the same is observed in case (1) until significant heat release has occurred). The flow patterns are visualized with the Q-criterion, where \( Q = 0.5 (\Omega_{ij} S_{ij} - S_{ij} \Omega_{ij}) \), with \( \Omega_{ij} \) and \( S_{ij} \) denoting respectively the antisymmetric and symmetric components of the velocity gradient tensor \( \frac{\partial u_i}{\partial x_j} \) [33], which are markers of the turbulent vortical structures. Close to top-dead-center, the flow undergoes significative change in its topology. Large scale Kelvin–Helmholtz toroidal vortices, generated downstream of the admission plane, are present at \( 0.94 t_{TDC} \) (Fig. 6a), to strongly cascade when the flow reaches the closing-cylinder wall, ending in a quite well developed turbulence at \( 1.07 t_{TDC} \) (Fig. 6c).

Table 1

| Case | \( T_{Ac}/T_o \) | \( t_{ig}/t_{TDC} \) | \( u/|U_o(t)| \) (%) | 3D/2D | Ignition location | Ignition regime |
|------|------------------|----------------------|----------------------|------|-------------------|----------------|
| Case (1) | 48 | 0.976 | 10 | 3D | Vortex core | Homogeneous |
| Case (2) | 52 | 1.134 | 10 | 3D | Shear layer | Spotty |
| Case (3) | 52 | 1.187 | 10 | 2D | Vortex core | Homogeneous |
| Case (4) | 48 | 0.970 | 30 | 2D | Shear layer | Spotty |

Figure 6. Iso-contour of Q-criterion \((Q = 15 \times 10^6 \text{ s}^{-2})\) colored by temperature, case (2). Flow goes from left to right.

(a) 0.94 \( t_{TDC} \)

(b) 0.99 \( t_{TDC} \)

(c) 1.07 \( t_{TDC} \)

Fig. 6. Iso-contour of Q-criterion \((Q = 15 \times 10^6 \text{ s}^{-2})\) colored by temperature, case (2). Flow goes from left to right.

Fig. 7. Pressure and temperature centerline plane. Case (2), \( t = 0.94 t_{TDC} \).

(a) Pressure

(b) Temperature
almost unaffected by heat losses at walls close to the admission plane, thus mainly evolving according to the global compression. This is also visible in the temperature snapshot (Fig. 7b), where cold fluid is entrained from the wall to be intensively mixed with the main flow, up to an almost uniform temperature zone, not yet affected by small scale fluctuations. At this instant in time, $\psi_T$, the temperature chemical source, is more than two orders of magnitude smaller than other RHS contributions of Eq.(7). The diffusive budget (term (i)) dominates over the highly wrinkled iso-temperature surfaces (Fig. 8a), with some occurrence of localized compression and dilatation (term (iii)) due to fine-scale turbulence motion (Fig. 8b). In some zones, these two terms are of same order of magnitude and compete to control the Lagrangian temperature time evolution. Still, at this particular time, the flow close to centerline and up to the first half of the cylinder is left unaffected by diffusion or local velocity divergence fluctuations and behaves as an adiabatic core. Outside of this core, local minimum of $\nabla \cdot \mathbf{u}$ are visible in Fig. 8b (inside circle in the iso-contour), directly related to a local temperature maximum visible in Fig. 7b.

The correlation between non-zero local flow divergence and low level of flow rotation dominated zones is evidenced in Fig. 9, taken shortly before ignition, where low $\nabla \cdot \mathbf{u}$ was observed for the full range of $Q$-values, whereas high positive or negative $\nabla \cdot \mathbf{u}$ mainly occur for very low $Q$-levels (i.e. outside turbulent flow structures). The correlation between a local temperature rise and a negative value of $\nabla \cdot \mathbf{u}$ is shown in Fig. 10, which also gives information on the level of temperature fluctuations. At the instant considered, just before ignition starts, all the points featuring temperature above 750 K are with $\nabla \cdot \mathbf{u} < 0$ and $\partial T/\partial t > 0$, according to Eq. (7).

At this stage, this preliminary analysis suggests that first ignition, controlled by local temperature rise, is likely to occur either, inside turbulent flow structure, which are thermally homogeneous in their core and somehow insulated avoiding large heat-loss with their surrounding, or, between these coherent structures, in local compression zones where $\nabla \cdot \mathbf{u} < 0$. Therefore, if ignition is to be wished within large scale rollers, they must have a life time large enough, typically much larger than the ignition time, to avoid being thermally affected in their core by wall heat transfer; a similar behavior was reported in the case of non-premixed mixture ignition within vortices [34].

### 3.2. Ignition phase

Figure 11 shows the temperature field in the transverse plane where the first significant chemical source is observed (i.e. where combustion is initiated) for both cases (1) and (2), featuring the same turbulence level but different ignition delays (Table 1). In case (1), ignition occurs in the second half of the cylinder, close to its top-end; in case (2), combustion starts in the first half of the combustion chamber, in the vicinity of the admission plane.
In the first case (Fig. 11a), featuring the shortest ignition delay, the sudden temperature rise (100 K above the adiabatic compression temperature) is visible uniformly over the south-west part of the section, in a flow zone where toroidal-vortices subsist, and also in some other areas of the same section, for instance in the north-east. High temperature fluctuations exist in the chamber at this time, as visible in the not yet fully burning zones (Fig. 11a), with three dimensional complex and convoluted temperature gradient patterns, which are rapidly smoothed out by the subsequent full ignition. The adiabatic compression drives here an almost homogeneous ignition that covers a flow zone populated by large scale flow structures. This behavior is observed in the representative temperature profile displayed in Fig. 12 (line), where multiple temperature maxima (localized volumes) are found together with a high temperature plateau (larger volume). Overall, all the points are ignited at the same instant in time and ignition in this case is controlled by temperature rise inside vortical structures.

In the second case (Fig. 11b), more time has elapsed before combustion starts. There, variability is much reduced and almost all the points are at the same thermodynamic state, see profiles in Fig. 12 (dash-line). In Fig. 11b, it is seen that ignition proceeds differently from the previous case, the very first temperature rise occurs in a small volume only. Very localized tiny differences in flow properties, eventually due to velocity divergence (term (iii)) outside remaining vortical structures, lead to the decisive temperature increase, as observed in Fig. 12 (dash-line) at \( x = 0.23 \). This is also illustrated in Fig. 13a, a cut in the centerline plane confirms that the place of ignition observed in Fig. 11b belongs to a well defined and quite small volume located on the north-west quadrant of Fig. 13a. This already ignited volume is also visible with a negative term (iii) in Fig. 13b, therefore representative of gas expansion due to burning (\( \nabla \cdot \mathbf{u} > 0 \)). To better seek out the role played by \( \nabla \cdot \mathbf{u} \) in ignition location, profiles of temperature and of term (iii) are taken along the white line shown over the iso-contours of Figs. 13a and b, in a zone that is not yet burning. A positive contribution of term (iii) associated to a local compression (\( \nabla \cdot \mathbf{u} < 0 \)) is visible in Fig. 13b and c with, at the same position, a temperature increase of 60 K adding to the global compression. A few instants later this zone is fully ignited. In the rapid compression machine simulations reported under these conditions, ignition is always very spotty, not all the points undergo ignition at the same instant in time, and they are distributed in the zone bordering vortical structures (Fig. 8b).

These two different ignition regimes are illustrated in Fig. 14, displaying an iso-surface of progress of reaction, corresponding to a temperature of about 1400 K for these two cases. In the first (Fig. 14a), ignition has occurred close to the top-end of the cylinder, within intense turbulence (see Fig. 7) and over a quite large flow volume; it is followed by strong pressure waves. In the second case (Fig. 14b), ignition is observed for at least three different locations; without significant pressure waves.

These basic mechanisms are now further investigated in two-dimensional simulations, which are useful to isolate the impact on the temperature budget of well defined flow structures, amplified in two-dimensional flows because of the lack of vortex breakdown.

4. Mechanisms analysis from 2D-flow

4.1. Two-dimensional cases

In two-dimensional simulations, the basic ignition mechanisms involved (inside or outside coherent structures) are still observed, but not for the same turbulence levels and chemistry conditions. Between 2D and 3D cases, it was decided to preserve the position in time of the instant of ignition with respect to top-dead-center (Table 1). The chemistry and turbulence conditions of the 3D case (2) are kept to build the 2D case (3), leading to the ignition time \( t_{\text{ig}} = 1.187 t_{\text{TDC}} \); but in 2D ignition first appears inside vortices (outside in 3D for \( t_{\text{ig}} < t_{\text{TDC}} \)). To reproduce in 2D ignition right before top-dead-center, keeping same chemical parameters than in
3D case (1) (Table 1), it was found necessary to increase the turbulence intensity at the inlet grid up to 30% of the bulk velocity, leading to the 2D case (4), there ignition first appears between coherent turbulent structures at $t_{ig} = 0.970 t_{TDC}$.

4.2. Ignition and propagation scenarios

Looking at the overall field, Fig. 15-a and -b show that the chemical source term (ii) is initiated inside vortices core in case (3) and outside vortices in case (4); very soon after ignition, the burning rate reaches its maximum inside (resp. outside) zones of pressure drops in case (3) (resp. case (4)) (Fig. 15c and d), which are here representative of coherent flow motion as confirmed by the iso-contour of Q-criterion (Fig. 15e and f). The temperature scalar dissipation rate, $\nu T = (k/C_p) j^2_{T}$, is maximum in the zones of intense mixing bordering vortices and is mainly associated to lower burning rates, because of heat exchange with places influenced by the cold-wall. In case (3), left in Fig. 15, the vortex cores appear to be thermally insulated from their environment and combustion preferably starts inside vortices. In case (4), turbulence fluctuations are much higher and it is local compressions that initiate burning; Fig. 16 is extracted from the simulation of case (4) at the very instant and place where combustion starts. The gas is pulled forward by two counterrotating vortices, with an acceleration due to streamline constriction; the compressibility prevents the volumetric flow rate from being exactly conserved, consequently the compressible bulk velocity between the vortices is less than an...
equivalent incompressible one, \( \frac{\partial \rho}{\partial t} > 0 \) and \( \nabla \cdot \mathbf{u} < 0 \), thus term (iii) is a source in Eq. (7).

The topology of the temperature field right before ignition has direct consequences on the pressure field after ignition; the pressure variation generated by ignition is of the order of \( \Delta P = 200 \) Pa in case (3) and \( 10^4 \) Pa in case (4). Pressure waves generated in case (4) are sustained and propagate, as seen in Fig. 17-right, they also shorten ignition delay and favor combustion when they travel to places which are close to burning. In the center of Fig. 17f, the passing of a wave emitted from a point in the north-east quadrant (Fig. 17d) fasten ignition. In the case (3) featuring almost homogeneous ignition inside vortices, the pressure rise is global without much visible discontinuities (Fig. 17-left).

The propagation of ignition was discussed by Zeldovich [1], along with the concept of spontaneous ignition wave. A dynamic coupling between the propagation of the ignition front and the pressure wave may occurs, with a mutual amplification up to the generation of a shock wave. The flow domain must be large enough for the amplification process to build up [35], and for much smaller volumes, as the one considered in the present rapid compression machine, strong acoustic waves can only be found.

A precise definition of the ignition delay \( \tau^*_i \) in the sense of Zeldovich’s analysis could be achieved from the chemical source term in the simulations, but this source implicitly depends on all flow
parameters evolving in space and time and it is difficult to track a $\tau_\gamma(\mathbf{x},t)$ distribution in the rapid compression machine with turbulence and temperature fluctuations. On the other hand, the ignition wave moves at the absolute temperature displacement velocity $\mathbf{u}_{\text{abs}} = \mathbf{u} + S_d \mathbf{n}$, where $S_d$ is the relative displacement speed of the temperature in the direction $\mathbf{n}$, normal to its iso-surface. $S_d$ may be defined from a field equation [36,37]:

$$S_d = \frac{1}{|\nabla T|} \frac{DT}{DT}. \quad (8)$$

With a given global temperature increase induced by compression, Eq. (8) confirms that the smallest the temperature gradients, the highest the speed at which the ignition iso-temperature surface propagates, even without flow motion, then quasi-volumic ignition may be reported. $S_d$, the displacement speed of the temperature field, as defined by Eq. (8), is thus an interesting candidate to quantify the speed at which ignition spatially develops inside a given volume and this option is here retained. It is essential to note in this analysis that high $S_d$ does not mean high flow velocities, in the limit case of quasi-homogeneous mixture at rest, $S_d$ would be close to infinity without flow propagation of any kind. Therefore, it is just an indicator of the speed at which the ignition temperature value spreads out in the flow domain.

In the literature [38], it was previously discussed how compressibility effects (i.e. $(1 - \gamma)\nabla \cdot \mathbf{u}$ in Eq. (8)) can lead to higher displacement speed of the front and must be included in $S_d$. In other words, a displacement speed based on the diffusive and reactive budget only, would not be fully relevant for auto-ignition studies in compressible flows.

Figure 18 presents scatter plots of $S_d$ vs $c = \sqrt{\gamma T}$, the speed of sound ($S_d$ is measured only where the burning rate is non-zero).
The temperature wave displacement velocity takes higher values in case (4) than in case (3). This is explained by the ignition mode associated to the temperature distribution and it is essential here to distinguish between 2D and 3D cases.

In case (3), in 2D flows the temperature globally increases inside vortices, which are separated by layers of intense heat-diffusion. The diffusive term \( i \) of Eq. (7) has a negative contribution to \( \frac{DT}{Dt} \) in the zone bordering coherent structures and \( S_d \) stays moderate, not allowing for a rapid ignition wave to develop between already hot spots. In case (4), ignition occurs in compressed zones within these diffusive layers, leading to various hot spots, surrounded by vortex cores, thus by zones weakly affected by heat-diffusion and featuring weak temperature gradients. Fast propagation of ignition is observed in these places weakly affected by heat-diffusion; one \( S_d \) point is even above the speed of sound in Fig. 18.

In the 3D cases studied above, places weakly affected by heat-diffusion are also promoting strong pressure waves, which are then more likely to be observed in case (1), featuring quasi-homogeneous ignition inside coherent vortices; while strong pressure waves cannot develop with larger ignition delays, associated to spotty ignition and a broader variety of temperature gradients.

### 4.3. Departure from PSR and canonical ignition regimes

The three terms of the temperature budget are plotted at different instants in time versus \( \frac{DT}{Dt} \) in Figs. 19 and 20, therefore vs their sum. In case (3) having combustion later than in case (4), turbulent stirring of the temperature iso-surface is well developed at the ignition time and the diffusive budget brings higher contribution than in case (4) (compare crosses spreading about the zero value in Figs. 19 and 20). This difference in heat-diffusion contribution at the ignition time was already mentioned above, when comparing the iso-temperature surface displacement speed \( (S_d) \). Concerning the dilatation term \( iii \) (squares), there is almost no deviation from a linear behavior in case (3), whose ignition is not controlled by this contribution; in contrary with case (4) close to ignition, there is some departure of this term from the linear response and the same is observed for the chemical source. Nevertheless, a global linear trend is seen in the plots.

Auto-ignition modeling in complex systems, as internal engines, has been tackled in the literature at many occasions from perfectly stirred reactors (PSR) (see for instance [39,40] and references therein), mostly assuming that the ignition sequence can be viewed as collection of PSRs at constant pressure, or constant volume. Under these conditions, according to Eq. (5), at constant pressure:

\[
\frac{T}{C_1 u} = \frac{DT}{Dt} \tag{9}
\]

and back in the equation for the temperature (Eq. (7)) neglecting the diffusive term \( i \), the usual constant pressure PSR temperature evolution is recovered.
Thus, if the flow conditions are constant pressure PSR like, the compressibility term \((iii)\) should behave linearly vs \(\frac{DT}{Dt}\) with a negative slope \(-\gamma - 1\) (in a constant volume PSR, \(\nabla \cdot \mathbf{u}\) would in fact imply a pressure change in the PSR), while the chemical source would also be linear, with a positive slope \(\frac{\gamma}{\rho C_p}\) at constant pressure and \(\frac{\gamma}{\rho C_p}\) at constant volume.

This is what is observed in Figs. 19 and 20 selecting the constant pressure approach; the same would be concluded at constant volume, with the same spreading of the points around a linear response having a different slope. The PSR response may thus be an interesting modeling approach. Nonetheless, to be accurate enough, the initial condition of the PSR should account for the small departure from the linear response, including local flow perturbations, visible in the spreading of the scatter plots. This point can be refined by directly comparing the progress of reaction against PSR responses.

Figure 21 shows the time evolution of \(c(x(t))\), the progress variable following one ignition kernel of case (4) in a lagrangian manner, i.e. on the maximum temperature trajectory. On the same graph, solutions of constant pressure PSRs (Eq. (11)) for different initial conditions taken along the \(c(x(t))\) DNS response are given. If the PSR initial state is taken too early before chemistry dominates (term \((ii)\)), perturbations in the DNS (mainly dilatation term \((iii)\)) have time to act before burning is initiated and the DNS solution deviates from the PSR one. However, for an initial state taken much closer to ignition, a perfect match between PSR and DNS is achieved. This suggests that PSR at constant pressure is an interesting approach to the modeling of auto-ignition in such turbulent flows, but to be at its best it should be calibrated according to local flow properties, accounting for the flow time-history in the selection of the initial PSR condition.

Similar conclusions concerning the key role played by flow time-history properties was recently reached analyzing a flow controlled chemistry tabulation based on residence-, engulfment-(stretch) and mixing-time [41]; specifically, the time-evolution of scalar concentration bounds within a coherent structure was calibrated. Transposed to the actual problem, Fig. 22 is a schematic summarizing what has been observed in the present simulations inside flow rollers. After the rapid compression, temperature within a given large scale flow structure evolves according to two characteristic times representative of mixing and flow engulfment, as described in [42]. The temperature first increases in the vortex core with the adiabatic compression, without being much unaffected by mixing with colder fluid due to wall, for a duration, or a vortex residence time that depends on local mixing and coherent-structure flow-engulfment intensity. If \(\tau_{ig}\), the chemical ignition delay is
short enough, ignition may occur within vortices core; for larger ignition delay, the temperature inside flow coherent structures is affected by mixing with colder fluid and the flow rollers may lost their preferential role as primary ignition sites, ignition will then start where local flow compressibility, or may be another mechanism in more complex systems, will ensure the local required thermodynamic conditions for combustion.

5. Summary

Large Eddy Simulation of an experimental set-up \[15,16\], in which a reactive mixture is rapidly compressed in a combustion chamber after passing through a turbulence-grid, have been performed with a fully compressible flow solver, using a structured mesh with immersed boundaries for modeling the cylindrical wall. After comparing with experiments the major flow properties, the chamber volume is downsized for Direct Numerical Simulation with single-step chemistry using about 70 million nodes and a resolution of 20 \(\mu\)m, but preserving the flow admission sequence properties.

Heat transfer at the wall rapidly promotes a weakly stratified temperature field and mechanisms controlling the birth of ignition under these conditions are analyzed. After the rapid compression, coherent flow structures are generated during the admission of the fuel-lean charge in the combustion chamber. The temperature distribution inside these structures evolves according to three phenomena: adiabatic compression, engulfment and mixing with colder fluid from wall boundary layers. Accordingly, a competition develops between the adiabatic compression, which increases the temperature of the volume of gaseous mixture, and, mixing with colder fluid from wall, which locally decreases fluid internal energy. Under these conditions, two major ignition scenarios have been recovered:

- For an ignition delay smaller than the time required for turbulent mixing to damp high temperature fluctuations between wall layers and the inside of coherent flow structures, the core of large-scale vortices is almost 'thermally insulated' and ignition will primary appear inside these flow rollers, which are homogeneously distributed over the flow domain, leading to a global and quasi-uniform ignition phenomena.
- When turbulent mixing has sufficiently influenced the flow before ignition, the starting of ignition will be controlled by very localized details of the flow topology, as for instance local compression zones between coherent structures, where the flow divergence is an additional source of temperature. Ignition is then found to be non-global, but rather scattered and spotty.

Depending on the temperature field right before autoignition, and in accordance with \[1\], after ignition has started two routes are found in the simulations leading to combustion spreading:

- Primary ignition may be followed by a rapid ignition wave, due to the propagation of pressure bursts, which can reduce local ignition delay from place to place, when traveling over the flow. This is mainly observed in the case of quasi-homogeneous ignition.
- In the case of quite intense diffusion of heat in the zone bordering vortices (large temperature scalar dissipation rate), as it is the case with spotty-ignition, the propagation of a strong ignition wave traveling throughout the flow has not been observed in the three-dimensional simulations.

Preliminary experimental results on this compression machine with combustion confirm these two scenarios, in terms of global versus localized ignition depending on fuel type \[43\]. It is worthwhile to keep in mind that the simulations did not include cool-flame effects, therefore these comparisons can only be made, focusing on the topology of the very first burning zones when ignition delays vary. Cool flame is usually pictured with two characteristic ignition delays, corresponding to the first small temperature rise and to the subsequent thermal runaway, occurring after a temperature plateau. In the context of these simulations, comparison can only be made against experiment concerning the appearance of the very first temperature increase due to combustion, whatever is the subsequent mechanism (immediate full ignition or temperature plateau before full ignition). Nevertheless, these observations reinforce the well-known and major role played by the flow topology after admission in combustion chambers of internal engines and the possibility of controlling the ignition regime through details of turbulence properties, found right after rapid compression. On the other hand, stratification in equivalence ratio may be also of premier importance to achieve ignition control \[44\].

Accounting for detailed chemistry and transport properties would certainly lead to much more complex ignition patterns, but the observations of the temperature distribution right before ignition would not be affected and these are small temperature variations which are known to have a profound impact on ignition; therefore the overall ignition scenarios may not be profoundly modified.

Still, the introduction of more detailed chemistry in such DNS based on real experimental devices, rather than on canonical flow problems, is a must for future works using three-dimensional simulations. Indeed, the comparison between three- and two-dimensional simulations revealed that for the same turbulence level, ignition regimes switch from one to the other; therefore three-dimensional vortex stretching seems to be of primary importance for DNS study of ignition in engine context and definitive conclusions may be difficult to reach with two-dimensional DNS of ignition (even including detailed chemistry). Notice also that in practical engines, the wall thermal boundary layers may not be the main source of thermal stratification of the charge and the extent, to which thermal stratification from sources other than wall boundary layers would alter some of above conclusions, is difficult to quantify without considering real engines configuration.

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the piston versus time, the first control volume may be written
\[ V_p(t) = \int_{t_0}^{t} \mathbf{U} \cdot \mathbf{n} dS. \] (A.2)

Under these hypotheses, for any control volume \( V(t) \) within the system, the conservation of mass reads:
\[ \dot{V}(t) = -\int_{\partial V} \mathbf{U} \cdot \mathbf{n} dS, \]
where \( \partial V \) denotes the wetted surface of the volume \( V(t) \). Applying Eq. (A.2) to \( V_p(t) + V^* \), the volume of the pre-compression chamber plus the dead-flow zone (Fig. 1), and to \( V_{cc} \), the volume of the combustion chamber, leads to:
\[ \dot{V}(t) = -\frac{1}{V_p(t) + V^*} \left( -\dot{x}_p(t) S_p + U_p(t) S_{cc} \right) = \frac{1}{V_{cc}} U_p(t) S_{cc}. \] (A.3)

With \( S_p = \pi D_p^2 / 4 \) and \( S_{cc} = \pi D_{cc}^2 / 4 \) (Fig. 1). From \( x_p(t) \), the position of the piston versus time, the first control volume may be written
\[ V_p(t) + V^* = S_p(x^* - x_p(t)) + V^*, \]
where \( x^* \) relates to the dead-flow volume \( V^* = |x|^2 S_p \). Then:
\[ U_p(t) = \frac{R_p}{1 + R_p} \left( \frac{D_p}{D_{cc}} \right)^2 x_p(t), \] (A.4)
with \( R_p = V_{cc}/\left( (\pi D_p^2)/4(x^* - x_p(t))/4 + V^* \right) \).

References