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LES4ICE 2012 - Large Eddy Simulation for Internal Combustion Engine Flows

LES4ICE 2012 - La simulation aux grandes échelles pour les écoulements dans les moteurs à combustion interne

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Application of LES for Analysis of Unsteady Effects on Combustion Processes and Misfires in DISI Engine

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Résumé — Application de simulation aux grandes échelles pour l'analyse des effets instationnaires de combustion et d'allumage raté dans les moteurs DISI — Les variations cycliques de la combustion affectent fortement les émissions de polluants, la consommation spécifique de carburant et l'efficacité. Les moteurs à combustion interne du type « *Direct Injection Spark-Ignition* » (DISI) sont particulièrement sensibles aux fluctuations cycliques de l'écoulement, de mélange et de combustion. Une analyse basée sur la simulation multi-cycle aux grandes échelles (LES, Large Eddy Simulation), ici dénommée « multicycle-LES », est utilisée afin de caractériser les effets instationnaires de combustion et les allumages ratés dans un moteur DISI. Une analyse qualitative de l'intensité des variations cycliques de la pression, de la température et de la fraction de masse de carburant dans le cylindre est présentée. La probabilité d'allumage incluant l'étude des allumages ratés est en particulier analysée. Finalement, l'effet du gaz résiduel sur la pression, la température et les allumages ratés dans le cylindre est discuté.

Abstract — Application of LES for Analysis of Unsteady Effects on Combustion Processes and Misfires in DISI Engine — Cycle-to-cycle variations of combustion processes strongly affect the emissions, specific fuel consumption and work output. Internal combustion engines such as *Direct Injection Spark-Ignition (DISI)* are very sensitive to the cyclic fluctuations of the flow, mixing and combustion processes. Multi-cycle Large Eddy Simulation (LES) analysis has been used in order to characterize unsteady effects of combustion processes and misfires in realistic DISI engine. A qualitative analysis of the intensity of cyclic variations of in-cylinder pressure, temperature and fuel mass fraction is presented. The effect of ignition probability and analysis of misfires are pointed out. Finally, the fuel history effects along with the effect of residual gas on in-cylinder pressure and temperature as well as misfires are discussed.

INTRODUCTION

Cycle-to-cycle variations of combustion processes strongly affect the emissions, specific fuel consumption as well as work output. Especially Direct Injection Spark-Ignition (DISI) engines are very sensitive to cyclic fluctuations within the combustion chamber which can result in different work output for consecutive engine cycles, high fuel consumption and high emissions. A misfire can be considered as one of the most extreme cases of cycle-to-cycle fluctuations. In order to characterize the highly unsteady in-cylinder phenomena the Large Eddy Simulation (LES) has proved to be a reliable method [1, 2]. With respect to Internal Combustion (IC) engines, recent review of LES applications can be found in [3-6] and references therein. Multi-cycle LES based analysis has been used for investigating the effects of both unsteady spray combustion processes and misfires for various configurations of the spark-plug. Previous investigations of authors [3, 7-10] could show that the mixture quality at the spark-plug in air-guided direct injection gasoline engines is strongly affected by the flow inside the combustion chamber. A direct correlation was shown between the probability of misfire and the occurrence of a lean mixture at the spark-plug at the point of ignition [7]. The unsteady effects of cycle-to-cycle variations on spray combustion were pointed out in [3, 7], where the authors focused attention on in-cylinder pressure fluctuations and influence of various ignition points on the flow field pattern. An attempt to define and characterize misfires along with partial burned cycles in DISI engine was provided in [7], where ignition probability and analysis of misfires were discussed for four different positions of the spark-plug without consideration of residual gases and fuel history effects.

The present paper extends the previous works of authors [3, 7-10] by focussing particularly on misfire analysis and accounting for the issue of residual gases. Thereby the effects of cycle-to-cycle variations of the flow and mixture preparation on combustion processes are accounted for. Finally, the impact of residual gases and fuel history effects are pointed out and compared with previously obtained data.

The paper is organized in the follow way. The next two sections provide detailed information about configuration of IC-engine under consideration and description of numerical method and different models used. The discussion of the main results is given in the next section. The summary is provided in the last section of the manuscript.

1 IC-ENGINE CONFIGURATION

The investigated configuration shown in Figure 1a represents a four stroke DISI IC-engine [11] with Variable Charge Motion (VCM) system. This is a realistic IC-engine with four canted valves, an asymmetric cylinder head and an asymmetric piston bowl. The VCM system controls the in-cylinder charge motion which enables controlled guidance of the fuel penetration towards the spark-plug. Engine speed is 2 000 rpm, compression ratio is 10.5. Isooctane (C_8H_{18}) liquid fuel is used in the two-phase flow investigation. The main parameters of the IC-engine are listed in Table 1. The valve lift curves are given in Figure 1b. Computational HEXA grid with the total number of control volumes equals to 320 000 shown in Figure 1c is generated by using Ansys ICEM CFD program and provides a mesh resolution in the range of 0.2-1.0 mm following [7].

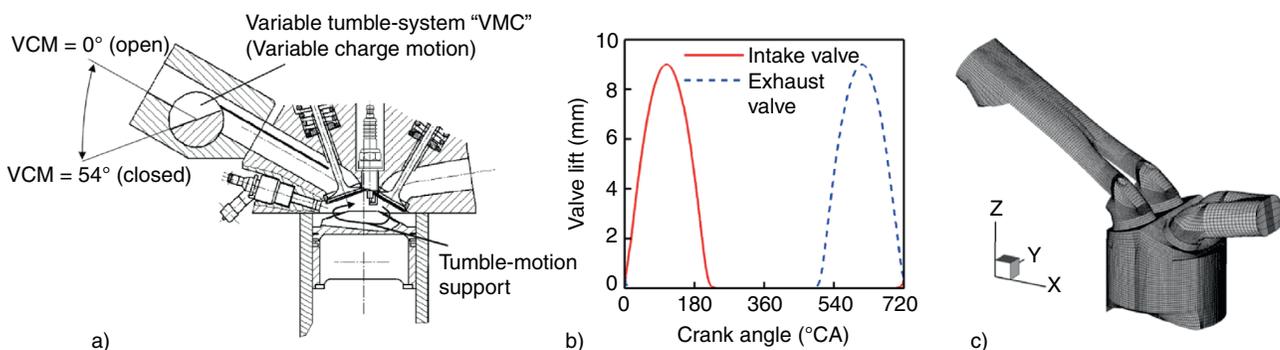


Figure 1

a) Configuration of the DISI engine [11], b) valve-lift curves, c) computational grid.

The computational grid shown in Figure 1c is used to perform LES simulations of the whole engine configuration with respect to non-reacting single-phase flow. The flow field is stored every 10° CA. Saved data make it possible to perform LES calculation of both non-reacting and reacting two-phase flows for various setting of injection and ignition parameters without repeating complete calculations of the whole IC-engine. As injection, mixing and ignition processes take place during the compression engine stroke, *i.e.* at closed intake and exhaust valves, the intake and exhaust ports were deactivated. The computational grid used for simulation of injection and combustion processes is shown in Figure 2a. Port

deactivation makes it possible to simplify and refine a computational grid, reduce the total number of cells and as a result, it reduces the computational costs.

The parameters of spray injection are tabulated in Table 2. The injector with an installation angle of 107° is located below the intake port (*Fig. 1a*). The fuel spray injection is initialized at 66.6 Crank Angle Degree (CAD) before Top Dead Centre (TDC), duration of injection is 21.6 CAD. For the spray simulation a hollow spray profile is used where a fuel is injected at a CONE angle with a spray thickness equals to parameter DCONE, see Table 2. The LES simulations involve the joint effect of both velocity cycle-to-cycle fluctuations

TABLE 1
Parameters of DISI engine

| Parameters | Values |
|---------------------|-----------|
| Bore | 85.0 mm |
| Stroke | 85.0 mm |
| Squish | 0.8 mm |
| Connecting rod | 141.0 mm |
| Engine speed | 2 000 rpm |
| Number of valves | 4 |
| Intake valve open | 336° ATDC |
| Intake valve close | 120° BTDC |
| Exhaust valve open | 120° ATDC |
| Exhaust valve close | 336° ATDC |

TABLE 2
Parameters of spray injection and ignition

| Parameters | Values |
|--------------------------|-------------|
| P_{inj} | 60 bar |
| T_{inj} | 393 K |
| Fuel | C_8H_{18} |
| Injection mass flow rate | 0.0076 kg/s |
| Start of injection | 66.6° BTDC |
| Duration of injection | 21.6 CAD |
| CONE | 40° ± 3° |
| DCONE | 12.5° |
| Ignition point | 45° BTDC |
| Duration of ignition | 15.0 CAD |

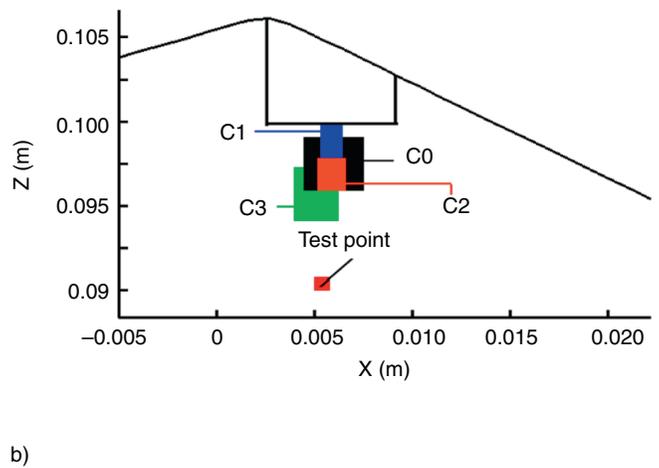
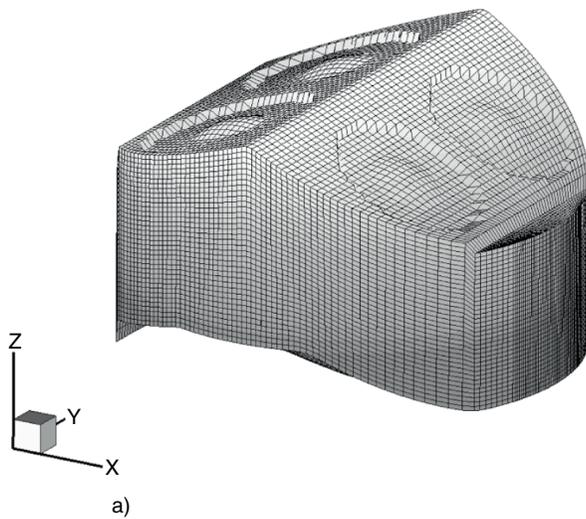


Figure 2

a) Computational grid for simulation of fuel spray injection, mixing, ignition and combustion processes, b) different configurations and locations of the spark-plug.

TABLE 3
Volumes of the spark-plug regions

| | | C0 | C1 | C2 | C3 |
|------------------------------|--------|-------|------|------|------|
| Coordinates of center point: | x (mm) | 6.0 | 5.9 | 5.9 | 5.2 |
| | y (mm) | 0.0 | 0.0 | 0.0 | 0.0 |
| | z (mm) | 97.5 | 98.8 | 96.9 | 95.7 |
| Volume (mm ³) | | 45.00 | 2.00 | 3.53 | 8.96 |

and variable spray boundary conditions [8, 9]. The variable spray boundary conditions are defined as a stochastic variation of the fuel spray angle CONE in the range of $40^\circ \pm 3^\circ$ corresponding to experimental findings [12] with the mean value equals to 40° and standard deviation equals to 1.89° .

The spark-plug region is defined as a volumetric region by setting of coordinates for two opposite corners. Different configurations of the spark-plug regions discussed in this paper are depicted in Figure 2b. Information about volumes of the considered ignition regions is collected in Table 3. The spark-plug region named C0 is taken as a reference.

Initial and boundary conditions for LES calculations are formulated as following. No-slip velocity boundary conditions at the walls and inlet/outlet pressure boundary conditions at the intake/exhaust ports are applied. The initial inlet/outlet pressure is set corresponding to the measured data described in [11]. Temperature of the piston, cylinder walls and cylinder head is set equal to 298 K. In order to estimate the effects of residual gases for consecutive engine cycles, two different series of LES calculations are considered: in the first series, the simulation of each next engine cycle begins from a fresh in-cylinder charge which does not contain the residuals from the previous engine cycles. In the second series, the IC-engine calculations involve the issue of residual gases, fuel history effects and the effects of unburned gases in the exhaust ducts.

The LES simulations of non-reacting single-phase flow covered 32 engine cycles obtained for the whole engine geometry including intake/exhaust ports, see Figure 1c. In additional calculations, since fuel spray injection and compression take places at closed valves, intake/exhaust ports were deactivated during simulation of injection and combustion processes. Ports deactivation made it possible to reduce the computational costs and allowed to perform LES simulation for above described 4 series of 32 engine cycles based on 32 engine cycles obtained for the whole engine configuration. Thereby, all LES calculations presented and discussed in present paper are carried

out on a computational grid shown in Figure 2a in the following range of CA: 45° Before Top-Dead Center (BTDC) until 45° After Top-Dead Center (ATDC).

2 NUMERICAL METHOD

The KIVA-3V software [13] used has found widespread applications for the simulation of IC-engine flows. The filtered governing equations are discretized using the finite volume method on an arbitrary hexahedral mesh applying the arbitrary Lagrangian Eulerian technique. KIVA-3V uses quasi-second-order upwind differencing for spatial discretization and the first order Euler scheme for calculating time derivatives. The mesh movement is the standard procedure implemented in KIVA-3V. The code extended to LES by integrating the standard Smagorinsky model among others is used to perform up to 32 consecutive engine cycles of reacting flows for each considered case. An application of developed parallelization strategy [10] enables to increase the number of samples allowing to perform LES of unsteady effects in an IC-engine with reasonable statistical accuracy.

The discrete droplet model of Dukowicz [14] with Lagrangian, computational particles that represent parcels of spray droplets with uniform properties is applied for the spray description. The KIVA-3V spray model has been calibrated by using a number of spray-bomb benchmark test cases described by Goryntsev *et al.* [7]. For the simulation of reacting two-phase flow a simple standard Arrhenius-based combustion model including 4 kinetic chemical and 6 equilibrium reactions is used together with an ignition model as described by Amsden *et al.* in [13]. In ignition model as provided in KIVA-3V, the internal energy in the specified ignition cells is increased during ignition by a factor of $(1.0 + XIGNIT \times DT)$ each time step as specified in [13], where XIGNIT is the reciprocal time constant for ignition energy addition to spark cells, DT is the time step. The energy deposition is terminated if the temperature in the ignition cells exceeds 1 600 K before the end of ignition. Thereby,

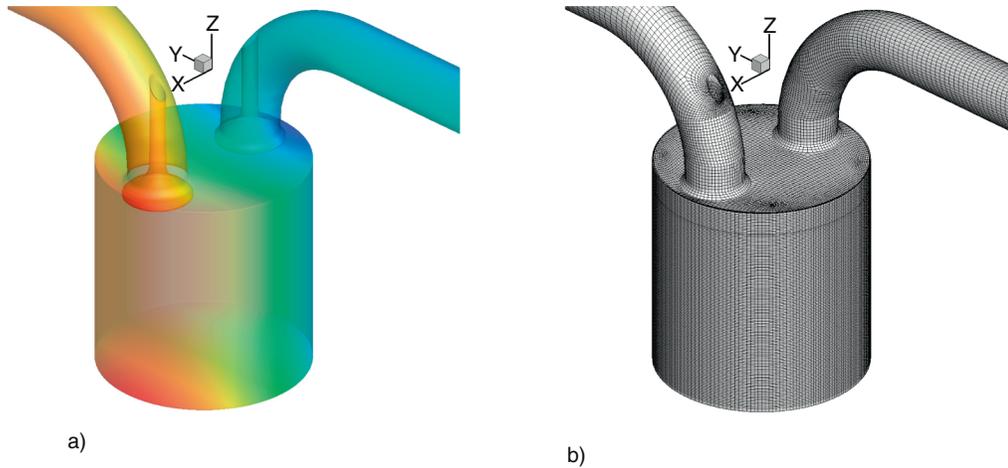


Figure 3
a) Geometry of TCC engine with 2-parallel valve, b) respective numerical mesh.

the amount of energy deposited within the spark-plug region depends on the volume. All ignition parameters are set the same for all considered cases.

3 LES ASSESSMENT

An attempt to verify and validate the results obtained in the complex reciprocating engine configuration using LES is provided in this section. For this propose an engine configuration with Transparent Combustion Chamber (TCC) shown in Figure 3a from Engine Combustion Network (ECN) [15] is taken to validate LES simulation for multiple cycles. The computational grid with 1 000 000 control volumes at BDC is presented in Figure 3b. The engine consists of relatively simpler geometry with 2-parallel valves. This configuration is designed especially to provide the validation data to assess the adopted numerical methodology. The detail engine parameters are listed in Table 4 and corresponding valve lift diagram is shown in Figure 4. In this particular case, LES simulations are performed up to 50 cycles and compared with available experimental data obtained by Sick *et al.* [16].

A comparison of the LES results for single-phase flow has been performed with available experimental PIV (Particle Image Velocimetry) data [15-17]. Measurement data were obtained using the same engine configuration under identical operating conditions. Figure 5 represents the comparison of in-cylinder flow field obtained in the cross section of the combustion

TABLE 4
Parameters of TCC engine

| Parameters | Values |
|-------------------|---------|
| Bore | 92.0 mm |
| Stroke | 85.5 mm |
| Squish | 11.0 mm |
| Engine speed | 800 rpm |
| Compression ratio | 10.0 |
| Number of valves | 2 |

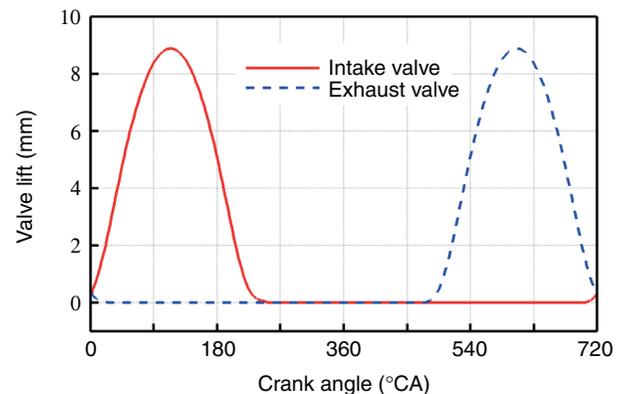


Figure 4
Intake/exhaust valve displacement profiles with engine crank angle for TCC engine.

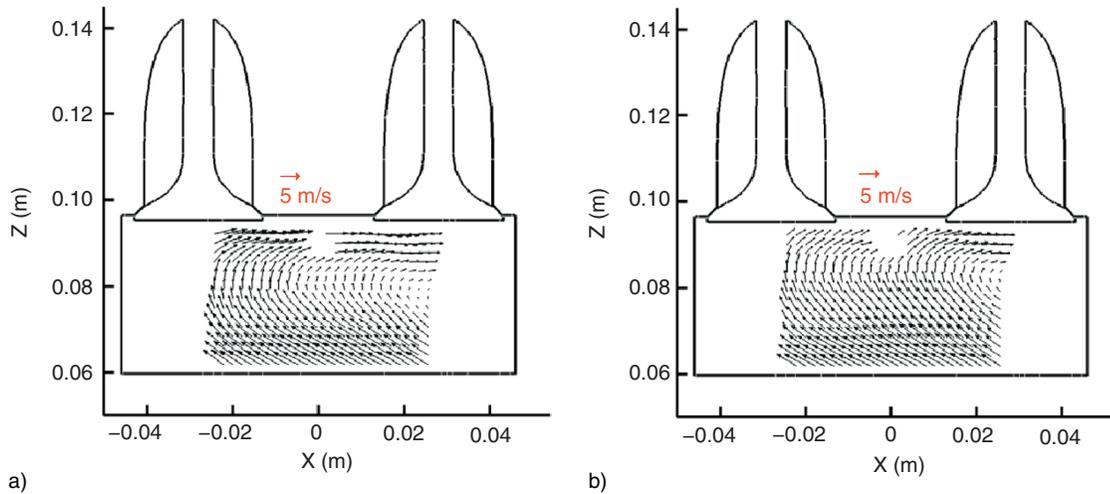


Figure 5

Velocity structure in the cross section of the combustion chamber during the compression stroke at $CA = 60^\circ$ BTDC. a) LES data averaged over 50 engine cycles, b) PIV data averaged over 3 000 samples.

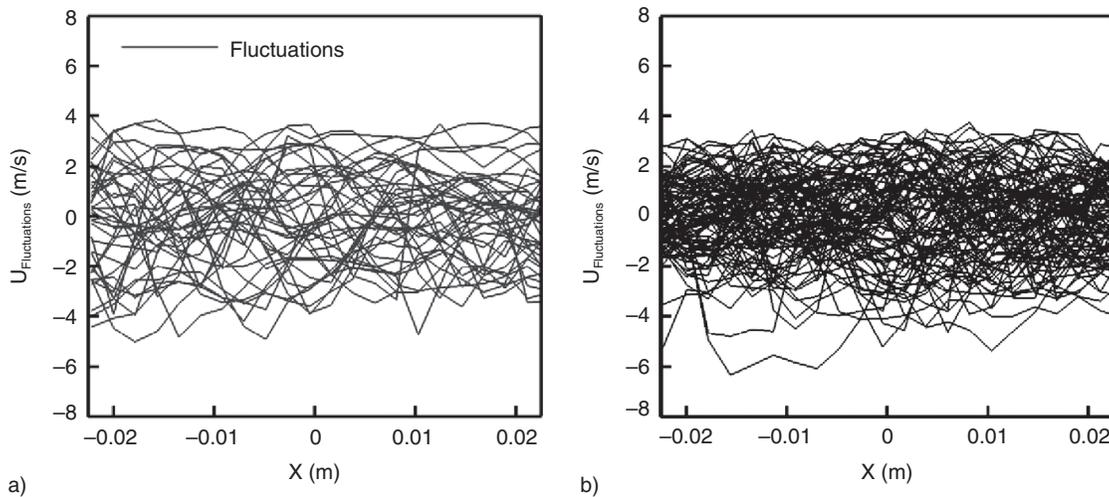


Figure 6

Velocity fluctuations ($z = 0.08$ m) at $CA = 60^\circ$ BTDC. a) LES data for 50 engine cycles, b) PIV data for 100 samples.

chamber at $CA = 60^\circ$ BTDC during the compression engine stroke. Inspection of the results reveals that LES predictions of the velocity flow field, *i.e.* velocity magnitudes, and the flow structure can be found in a good agreement with PIV measurement. To assess the

LES capability in terms of flow cyclic variability for multiple and consecutive engine cycles, velocity fluctuations are plotted in Figure 6. The compared LES results with PIV measurement show the same order of ± 4 m/s of velocity fluctuations.

4 RESULTS AND DISCUSSION

The present work provides an analysis of the unsteady effects on spray combustion processes and misfires in DISI IC-engine shown in Figure 1 as well as estimation of the impact of residual gases and fuel history effects. The multi-cycle LES covered 32 consecutive engine cycles for each considered configuration. The effects of various configurations and locations of the spark-plug regions on evolution of spray combustion processes and misfires are discussed. A qualitative analysis of the intensity of cycle-to-cycle variations of in-cylinder velocity, mass fraction, pressure and temperature is provided. Finally, comparisons of in-cylinder pressure, temperature, fuel mass fraction and velocity for cases with and without accounting for the fuel history effects based on analysis of 20 engine cycles are pointed out.

4.1 Characterization of Full-, Partly- Burned Engine Cycles and Misfires

At the time of ignition, the ignitable mixture near the spark-plug is mainly formed as a result of interaction between fuel spray jet and in-cylinder charge (tumble) motion which arises during the intake stroke. This interaction leads to realization of various conditions of air-fuel composition including fuel-lean, stoichiometric and fuel-rich mixtures. Unsteady effects like velocity cycle-to-cycle fluctuations along with variable spray conditions play an important role in formation of ignitable fuel-air mixture and can strongly affect the ignition processes. Thereby, cycle-to-cycle variations of in-cylinder flow can be considered as the most likely reason for realization of various conditions for combustion processes including full-, partly- burned cycles and misfires.

Figure 7 demonstrates the instantaneous and averaged profiles as well as the intensity of cyclic variations inside the combustion chamber for in-cylinder velocity (left) and temperature (right), respectively. Data are obtained from 32 consecutive engine cycles and correspond to the end of compression stroke, where combustion process takes place, at crank angle equals to 15° BTDC. Instantaneous, averaged velocity and temperature profiles are obtained along the line marked "A" which is located below the spark-plug at $z = 0.09$ m. There is only effect of velocity cyclic variations taking into account, *i.e.* the initial and boundary conditions for the fuel spray injection as well as ignition process are kept identical for the results presented in Figure 7. Hence, we can conclude that velocity cycle-to-cycle fluctuations result in the cyclic variations of the temperature field.

Evolution of instantaneous and mean in-cylinder parameters is presented in Figure 8 as a function of

crank angle for cases C0-C3. Based on 32 consecutive engine cycles, the mean in-cylinder velocity, fuel mass fraction, temperature and pressure curves are calculated separately for full burned (red lines) and partly burned (green lines) cycles as well as for misfires (blue lines). As it can be seen from data presented in Figure 8, in the cases of C0 and C3 only full- and partly- burned cycles are realized. At the same times, in cases C1 and C2 misfires were detected along with realization of full- and partly- burned cycles.

In order to distinguish full burned, partly burned and misfire cycles the instantaneous in-cylinder pressure values especially at the end of compression stroke obtained for consecutive engine cycles are analyzed. For example, in Figure 8d (case C1) the set of engine cycles with pressure values, similar to the single-phase represents the misfires (neighborhood of a blue line). The set of cycles with highest values of pressure characterizes the full burned cycles (near red line). The set of cycles with values in between full burned and misfires represents the partly burned cycles (near green line).

For case C0 (Fig. 8), almost all considered cycles are recognized as full burned (28 cycles) and only 4 partly burned cycles are detected. The mean velocity curve obtained based on full burned cycles is similar to the velocity curve which characterizes partly burned cycles as depicted in Figure 8a. Minor distinctions in fuel mass fraction and temperature curves (Fig. 8b, c) are found in the range of $CA = 40^\circ - 10^\circ$ BTDC. The in-cylinder pressure reaches the maximal value of 3.85 MPa for full burned cycles, while for partly burned this value does not exceed 3.40 MPa as can be seen in Figure 8d.

In contrast to C0, in the case of C1 all types of engine cycles including full burned (5 cycles), partly burned (8 cycles) and misfires (19 cycles) are realized. Large number of misfires obtained in this case can be explained by formation of nonflammable fuel-air composition near the spark-plug region at the time of ignition due to the strong cycle-to-cycle fluctuations of fuel mass fraction and relatively small volume of the spark-plug used in the case of C1. Fuel mass fraction under misfires is almost constant at the end of compression stroke at $CA = 45^\circ$ BTDC towards TDC as depicted in Figure 8b for case C1. Unburned engine cycles are characterized by low temperature (Fig. 8c, blue line) and total loss of in-cylinder pressure (Fig. 8d) at TDC. While full- and partly- burned cycles at TDC provide the in-cylinder pressure in the order of 3.3 MPa and 2.5 MPa, respectively, the mean in-cylinder pressure under misfires is less than 2.0 MPa. In-cylinder temperature at the end of compression stroke reaches 2 400 K for full burned cycles, 2 080 K for partly burned cycles and 750 K for misfires.

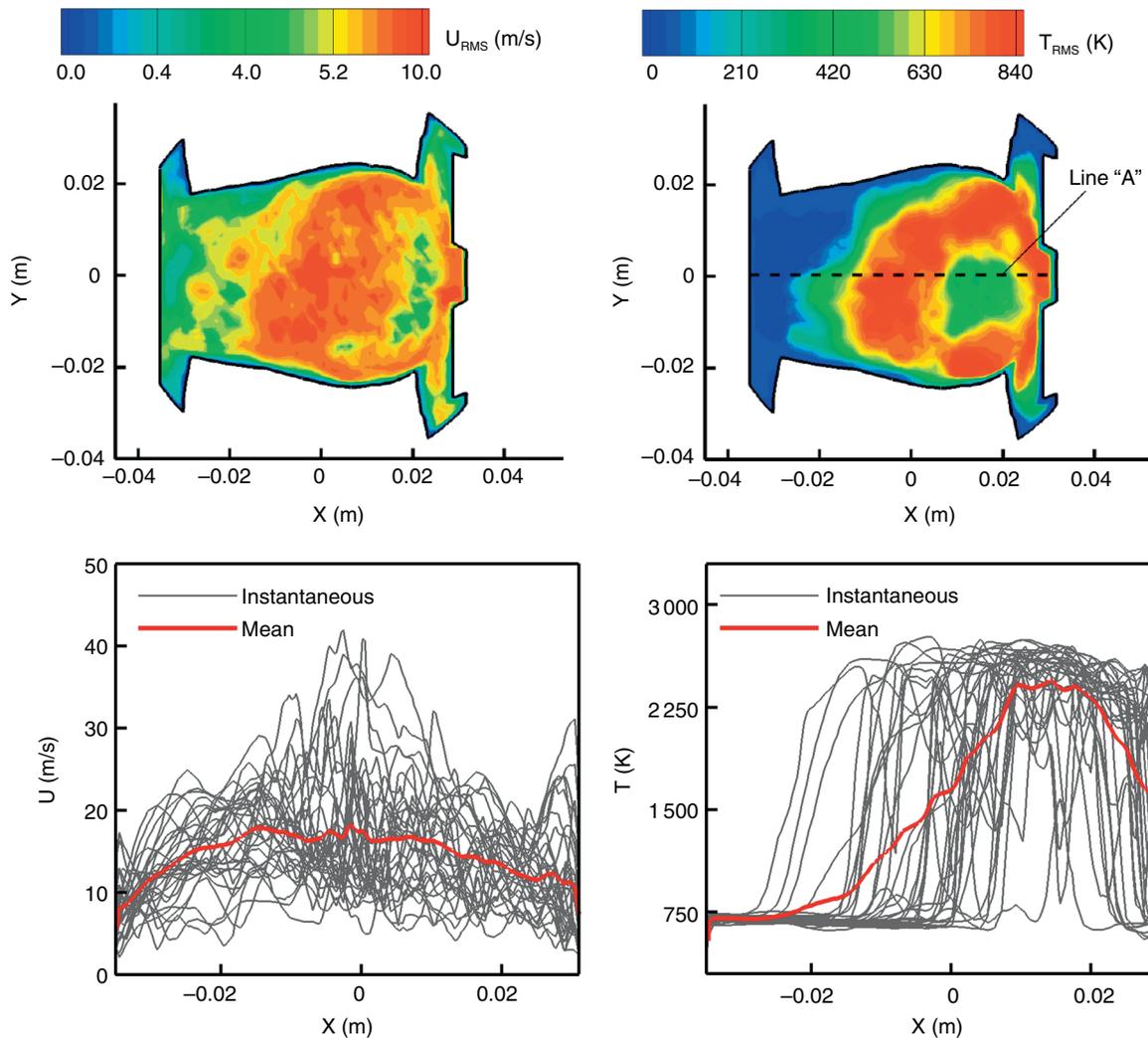


Figure 7

Standard deviation (top) and instantaneous and mean profiles (bottom) of velocity (left) and temperature (right) in the XY-section of the combustion chamber at $CA = 15^\circ$ BTDC. Profiles obtained at $z = 0.09$ m, position of the spark-plug corresponds to case C0.

In case C2, 16 full burned, 8 partly burned and 8 misfires are detected. This case gives values for in-cylinder temperature and pressure at TDC, similar to the case C1. In the case of C3 only, full- (29 cycles) and partly-burned (3 cycles) cycles are realized. The in-cylinder temperature and pressure at TDC are slightly low compared to the corresponding values obtained in the case of C0.

4.2 Influence of the Various Spark-Plug Configurations on Cycle-to-Cycle Fluctuations

Influence of different positions as well as volumes of the spark-plug on distribution and intensity of velocity and temperature cyclic variations is discussed in

this section. Figure 9 demonstrates the rms values of velocity (a, b) and temperature (c, d) obtained in the cross and perpendicular sections of the combustion chamber, respectively. Presented data correspond to $CA = 10^\circ$ BTDC and cover four configurations of the spark-plug described in Table 3 and shown in Figure 2b.

A rather uniform velocity flow field, obtained in case C0 and C3, reveals established homogenous cycle-to-cycle variations (*Fig. 9a, b*) with up to 10 m/s deviation from the mean velocity. At the same time the flame kernel continues to spread through the combustion chamber and the area with maximal intensity of temperature cycle-to-cycle fluctuations is achieved at the flame front

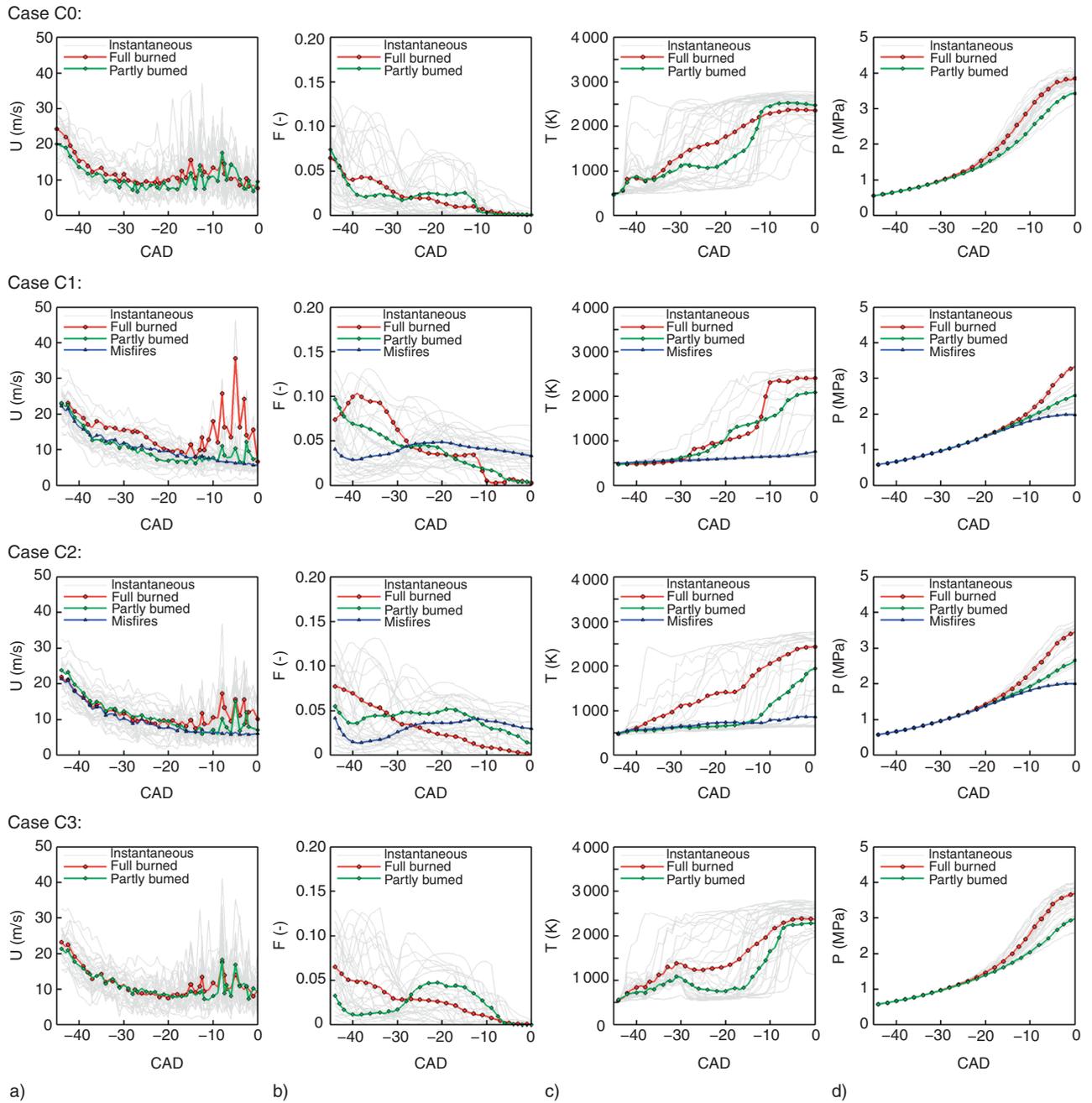


Figure 8

a) Evolution of mean in-cylinder velocity, b) fuel mass fraction, c) temperature and d) pressure obtained at the test point (Fig. 2b) under full burned (red), partly burned (green) and unburned (blue) conditions.

as depicted in Figures 9c and 9d for cases C0 and C3, respectively. For cases C1 and C2, where mostly partly- and un-burned engine cycles are realized, the intensity of velocity cyclic variations is rather small compared to the cases C0 and C3. The maximal values of velocity cyclic variations can be found at the centre of in-cylinder tumble motion as it is illustrated in Figure 9 (cases C1 and

C2) while the region with highest temperature cyclic variations is located at the center of the flame kernel.

4.3 Influence of Residual Gas on In-Cylinder Parameters

The instantaneous, mean and standard deviation of fuel mass fraction, velocity, temperature and in-cylinder

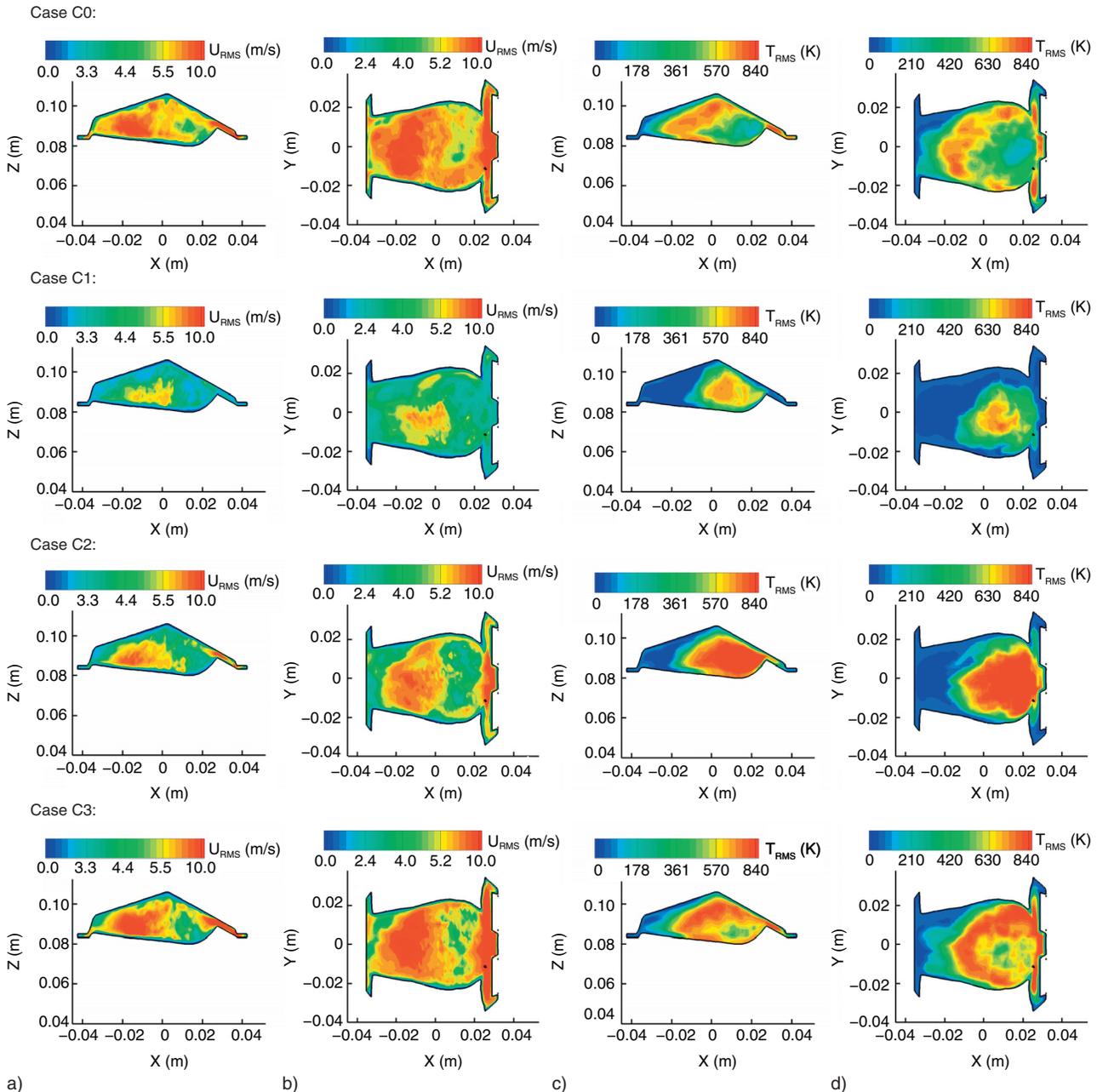


Figure 9

Location and intensity of velocity (a, b) and temperature (c, d) cycle-to-cycle fluctuations in the ZX ($y = 0.0$ m) and XY ($z = 0.09$ m) sections of the combustion chamber at CA = 10° BTDC.

pressure curves as a function of crank angle are given in Figure 10 for following cases:

- the fuel history effects and residual gases are not considered (Fig. 10, left). In this case simulation of each new engine cycles starts from a fresh in-cylinder flow field which does not contain information about fuel and unburned gases from previous engine cycles;

- simulation of consecutive engine cycles involves fuel history effects and residuals from previous engine cycles (Fig. 10, middle);
- Figure 10, (right) shows direct comparison for various in-cylinder parameters between above mentioned cases.

The results shown in Figure 10, (right) demonstrate relatively weak influence of residuals on mean fuel mass

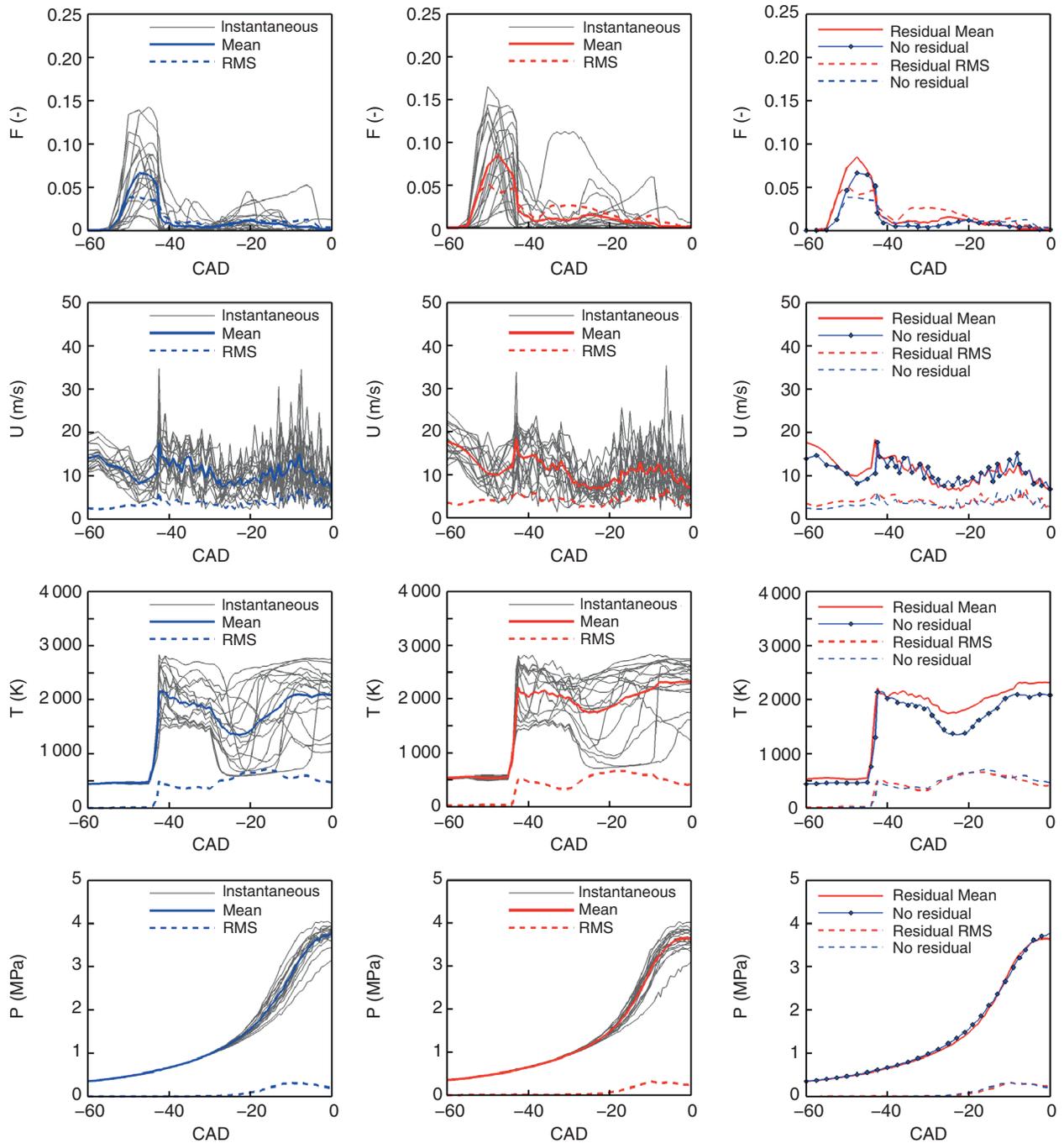


Figure 10

Instantaneous, mean and standard deviation of in-cylinder parameters. Case which does not contain residuals from the previous engine cycles (left), case which involves the fuel history effects (middle) and direct comparison between these cases (right).

fraction, velocity, temperature, pressure and their fluctuations. Taking into account residual gases, it gives slightly higher mean temperature towards TDC as

depicted in Figure 10, (right). At the same time values for mean and standard deviation of in-cylinder pressure are similar in both considered cases.

CONCLUSION

The multi-cycle LES based analysis covered up to 32 consecutive engine cycles for all cases under consideration. Four different configurations of the spark-plug are analyzed. Obtained results clearly show an evident unsteady effect, especially an impact of cycle-to-cycle variations not only on the flow field but also on the ignition processes and combustion through the temperature. The present investigation further emphasizes the issues of detection, characterization and prediction of misfires in a direct injection IC-engine in accordance with other previous works. Misfires can occur under various conditions such as hard loading, high engine speed, speed up or cold start conditions. It was shown that the location and configuration of the spark-plug plays an important role in initiation of misfires. Different locations of the spark-plug region strongly impact on the intensity of velocity and temperature cycle-to-cycle fluctuations and their distribution inside the combustion chamber. The described above processes were discussed in terms of mean and standard deviation of temperature, velocity, pressure and fuel mass fraction.

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