Simulation and comparison of diesel mixture formation at different fuel injection advance angles

Xiaolu Li, Jianguo Xing, Tao Hong

***Abstract*—**This paper simulates the density and temperature fields in the process of mixture formation with two combustion modes in a Diesel engine by adjusting its fuel injection advance angle. The computational simulations and experiments show that in the normal combustion mode, the density and temperature of mixtures change greatly during the injection so that there are premixed combustion and diffusion combustion simultaneously, which results in high nitrogen oxide and smoke emissions, but low carbon monoxide and hydrocarbon emissions. Homogeneous charge compression ignition combustion takes place by early-injection to form the stratified homogeneous mixture, which results in very low nitrogen oxide and smoke emissions, but high carbon monoxide and unburned fuel emissions.

***Keywords*—**Computational simulation, Diesel engine, Mixture, Injection, Homogeneous charge compression ignition

I. Introduction

THE global environment protection and energy conservation provide strong encouragement to develop more advanced technologies for high efficiency of engine combustion. For recent ten years, the homogeneous charge compression ignition (HCCI) combustion is becoming the research hotspot in the internal-combustion engine field [1]–[5]. Its features are multispot ignition without flame propagation, and low-temperature combustion without distributed heat release [6]. However, the main combustion mode of normal Diesel engine is the diffusion combustion, which can't resolve the contradiction between smoke and nitrogen oxide (NO_x) formation conditions, and this usually results in producing a lot of poisonous NO_x and smoke to environments and human beings [7]. HCCI combustion can reduce NO_x and smoke emissions simultaneously, but produce high carbon monoxide (CO) and hydrocarbon (HC) emissions.

There are a lot of studies about HCCI combustion, including its experiments and numerical computations [8]–[12] This paper obtains a two-stroke Diesel engine emissions and thermal efficiency in two combustion modes (normal combustion and HCCI combustion) by adjusting its fuel injection angle, and simulates and compares the process of its mixture formation by adjusting advanced computational models for the first time. All these are helpful to disclose the normal combustion producing high smoke and NO_x emissions simultaneously, and illuminate HCCI combustion having low smoke and NO_x emissions.

II. Experimental Bench and Parameters

A. Experimental bench

The computational simulation and experiment are completed on a 1E150C Diesel engine. The engine test bench is shown as Fig.1.

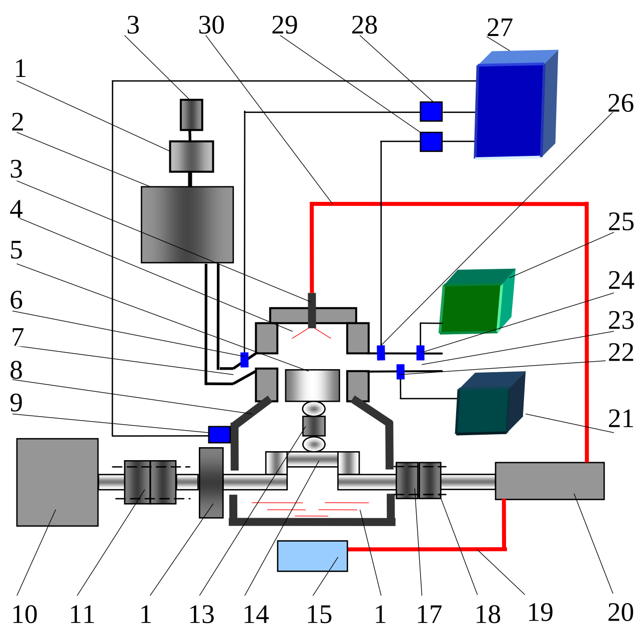

Fig.1 Schematic of engine test bench

1-Compressor, 2-Stable pressure box, 3-Injector, 4-Combustion chamber, 5-Piston, 6-Inlet air pressure sensor, 7-Inlet port, 8-Engine, 9-Crankshaft position sensor, 10-Hydraulic

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dynamometer, 11-Coupling shaft coupling, 12-Fly wheel, 13-Connecting rod, 14-Crankshaft, 15-Fuel mass flow meter, 16-Lubricating oil, 17-Joints for adjustable fuel delivery advance angle, 18-Connecting bolt, 19-Fuel pipe, 20-Fuel pump, 21-Smoke meter, 22-Probe for smoker, 23-Exhaust port, 24-Probe for five gas analyzer, 25-Five gas analyzer, 26-Exhaust pressure sensor, 27-Data acquisition system, 28&29-Charge amplifier, 30-High pressure fuel pipe, 31-Motor

In its normal combustion mode, the specification of the nozzle is $6\times\Phi0.25\times150^{o}$, and the fuel injection advance angle is 35 ^{o}CA BTDC (crank angle before top dead center). In HCCI combustion mode, the fuel injection advance angle of early-injection is 82 ^{o}CA BTDC, and the spray-angle is small as possible in order to avoid fuel impinging wall. Simultaneously, for better spray and more lean mixture, more nozzles should be manufactured at the tip of injector, so its specification is $6 \times \Phi0.25 \times 90^{o} + 4 \times \Phi0.18 \times 45^{o}$. The injection durations of these two combustion modes are 25 ^{o}CA.

B. Experimental Parameters

Engine parameters, operating parameters and calculating parameters are shown in Table 1.

Table 1 Engine Conditions

Parameter	Value	Parameter	Value
Cylinder diameter / mm	150	Scavenging port shape	Circular
Stroke/mm	225	Scavenging port diameter / mm	30
Connecting rod length / mm	450	Scavenge port open / ^{o}CA	+121.8 ATDC
Compression ratio	15	Scavenge port close / ^{o}CA	-121.8 ATDC
Combustion chamber	Shallow ω	Fuel injection temperature / K	350
Exhaust port number	3	Fuel quantity per cycle / g	0.117
Exhaust port shape	Rectangle	Injection pressure / MPa	20
Exhaust port wide / mm	30	Injection duration / ^{o}CA	25
Exhaust port high / mm	63	Fuel molecular formula	C_7H_{16}
Exhaust port open / ^{o}CA	+109 ATDC[a]	Rate / rpm	450
Exhaust port close / ^{o}CA	-109 ATDC	Scavenging pressure / kPa	111.7
Scavenging port number	6	Scavenging temperature / K	310

[a]ATDC: after top dead center.

The emissions of NO_x, HC and CO are tested by AVL Company's five gas analyzer Di Gas4000Light, and the smoke densities are measured by a full-automated FBY-200 smoke meter. The output power of the engine is calculated based on the data of engine torque and speed measured directly by the D650 hydraulic dynamometer and magneto-electrical speed sensor, respectively, while the brake thermal efficiency by using the data of engine output power and data of fuel consumption calibrated by the FCM-04 mass flow meter.

The accuracies of measurements and uncertainties in the calculated results are shown in Table 2.

Table 2 Accuracies of measurements and uncertainties in the calculated results

Measurements	Accuracy	Calculated results	Uncertainty
Torque	± 0.5 % FSR	Smoke	± 0.10 FSN
Speed	± 0.5 % FSR	Fuel consumption	± 0.2% FSR
Cylinder pressure	± 0.8 % FSR	Power	± 1.25 %
NO_x	± 1 ppm	Brake mean effective pressure	± 1.8 %
HC	± 1 ppm	Brake thermal efficiency	± 1.5 %
CO	± 0.01 %		

III. Computational Models and Conditions

A. Computational Models

Three-dimensional model of in-cylinder flow is based on classic fluid dynamics, namely the continuity, momentum and energy equations. Simulation of in-cylinder turbulence is completed by two equation models below as the turbulent kinetic energy equation (1) and the turbulent kinetic energy dissipation rate equation (2).

$$\frac{\partial \rho k}{\partial t} + \nabla\cdot(\rho\vec{u}k) = -\frac{2}{3}\rho k\nabla\cdot\vec{u} + \sigma:\nabla\cdot\vec{u} + \nabla\cdot[(\frac{\mu}{\mathrm{Pr}_k})\nabla k] - \rho\varepsilon + \dot{W} \tag{1}$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla\cdot(\rho\vec{u}\varepsilon) = -(\frac{2}{3}C_{\varepsilon 1} - C_{\varepsilon 2})\rho\varepsilon\nabla\cdot\vec{u} + \nabla\cdot[(\frac{\mu}{\mathrm{Pr}_\varepsilon})\nabla\varepsilon] + \frac{\varepsilon}{k}[C_{\varepsilon_1}\sigma:\nabla\cdot\vec{u} - C_{\varepsilon_2}\rho\varepsilon + C_s\dot{W}_s] \tag{2}$$

where ρ is the total mass density, k the turbulent kinetic energy, t the time, $\vec{u}$ the velocity, σ the viscous stress tensor, μ the first coefficient of viscosity, ε the turbulent kinetic energy dissipation rate, $\dot{W}_s$ the source term arise due to interaction with the spray, Pr_k the Prandtl number of k, and Pr_ε the Prandtl number of ε, C_{ε_1}, C_{ε_2}, C_{ε_3}, C_s, Pr_k and Pr_ε are constant, which are 1.44, 1.92, -1.0, 1.5, 1.0 and 1.3 respectively. The dispersion droplet model (DDM) is used to simulate the process of fuel spray, which is consisted of disperse particles. The spray liquid model includes the flow, breakup, collision and evaporation sub-models [13], while the combustion model is the turbulence/chemistry interaction model which uses the Partially Stirred Reactor approach [14]. An arbitrary Lagrangian-Eulerian (ALE) formulation is employed to resolve these equations.

B. Computational Conditions

The schematic of calculation grid is shown in Fig.2. Calculation starts at 121 ^{o}CA BTDC. In the calculation process, n-heptane is instead of diesel fuel [15]. When simulating the HCCI combustion, the cylinder wall temperature is assumed as 400K, cylinder top temperature 410K, and piston temperature 420K. While simulating the normal Diesel combustion, the cylinder wall temperature is assumed as 420K, cylinder top temperature 440K, and piston temperature 460K. The exhaust gas pressure is tested by a Kistler's 4045A5 low voltage sensor and 4618A0 charge amplifier. The exhaust gas pressure is shown in Fig.3. The scavenging pressure is a constant value as 111.7 kPa. All these are the boundary conditions of calculation.

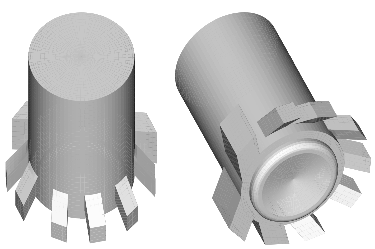

Fig.2 Schematic of computational grid

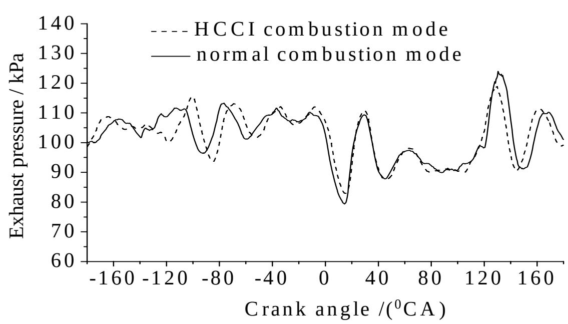

Fig.3 Exhaust gas pressure

IV. EXPERIMENT RESULTS AND ANALYSIS

In the experiment, the fuel consumption and rate is invariable. The experiment results are shown in Table 3, where p_e is the average effective pressure, η_{et} the effective thermal efficiency. In the normal combustion mode, there are more NO_x and smoke emissions, volume fraction of NO_x is 652×10^{-6}, and smoke is 0.5 Bosch. The formation condition of NO_x is high temperature and rich oxygen while the formation condition of smoke is high temperature and lean oxygen. In the normal combustion mode, diffusion combustion is the main combustion mode, and exist the formation condition of NO_x and smoke in the cylinder simultaneously. Owing to high temperature, there are less CO and HC emissions. In this combustion mode, the thermal efficiency is 31.32%.

Table 3 Experimental results

Combustion mode	Normal combustion	HCCI combustion
$\varphi_{NOx}\times10^{-6}$	652	0
Smoke / Bosch	0.5	0
$\varphi_{HC}\times10^{-6}$	10	65
φ_{CO} / %	0.01	0.32
p_e / MPa	0.47	0.28
η_{et} / %	31.32	18.66

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In HCCI combustion mode, owing to early-injection, the stratified homogeneous mixture is formed and burned at many points, which cause the peak temperature lower to prevent NO_x and smoke formation. In this experiment, there is none of these two emissions. Due to early-injection, the fuel impinges the cylinder wall, which results in high unburned fuel emissions. This is consistent with the experimental observation. In addition, CO and HC emissions are higher than normal combustion mode's. It is these unburned emissions resulting in low engine thermal efficiency, 18.66%. Certainly, the low thermal efficiency may also because of an advancing burning before the top dead center.

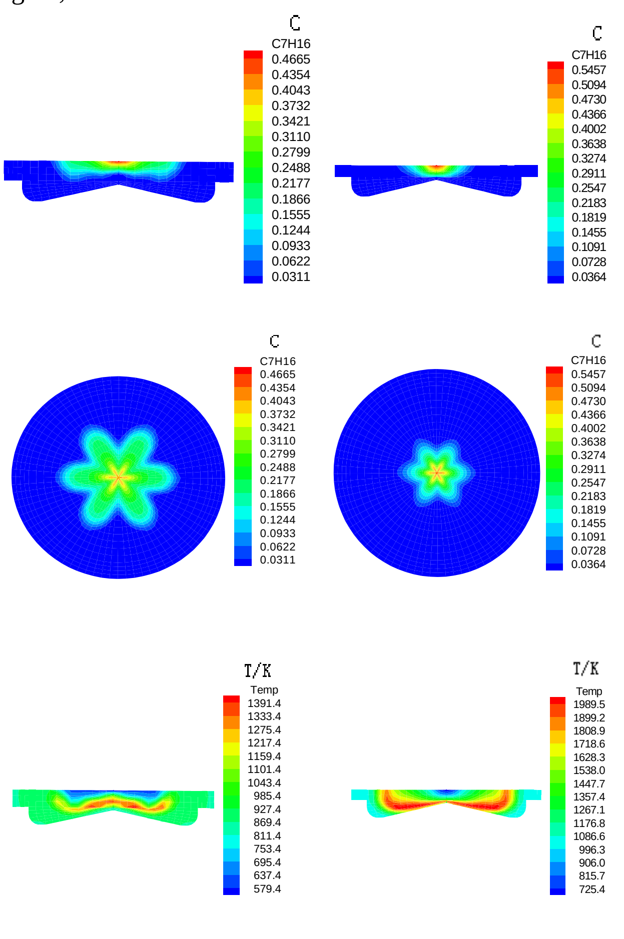
V. CALCULATION RESULTS AND ANALYSIS

A. Formation of Mixture in Normal Combustion Mode

This part simulates the density and temperature fields in the process of mixture formation with the normal combustion mode in a Diesel engine, the results are shown in Fig.4.

The unit of fuel density is mole fraction, and the unit of temperature is K. Injection starts at 35 ^{o}CA BTDC, and terminates at 10 ^{o}CA BTDC. The injection duration is 25 ^{o}CA.

Concentration and temperature fields at 16 ^{o}CA after the start of injection are shown in Fig.4(a). There are rich mixtures near the nozzle, due to fuel just leaving the nozzle. The fuel of this local part is unburned, where its temperature is about 750K. In the middle and front parts of the fuel injection, by air entrainment, the mole density of fuel is less than 0.25. The temperature field shows that the maximum temperature is around 1300K in the middle and front of injection. This also explains why combustion is very strong in this phase, which matches with the piston shape. Its mole fraction is 0.03 ~ 0.25, and the air equivalence ratio less than 0.6. It is obvious that the diffusion combustion is the main combustion mode of normal Diesel engine, namely "fire containing fuel" form. In other parts of combustion chamber, the temperature is about 1000K. Concentration and temperature fields at 1 °CA before the end of injection are shown in Fig.4(b). As the injection has almost completed, the injection distance is short. The region of high temperature is enlarging, and the maximum temperature near 2000K. The high temperature in the expanded region promotes the NO_x and smoke formation. Therefore, there are high NO_x and smoke emissions in the normal temperature combustion mode. As shown in Fig.4(b), the in-cylinder average temperature is a high value of 1100K at 11 °CA BTDC. With piston moving up and fuel combustion, the temperature is higher, so the CO and HC emissions are low.

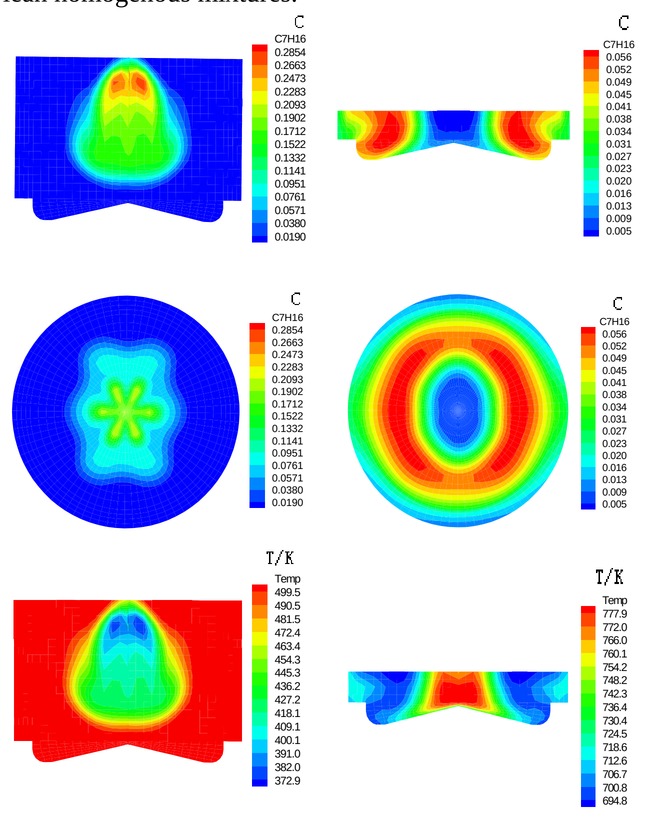


(a) 19 °CA BTDC (b) 11 °CA BTDC

Fig.4 In-cylinder fuel concentration and temperature fields in the mixture formation process under the normal combustion mode

B. *Formation of Mixture in HCCI Combustion Mode*

The simulation results of fuel concentration and temperature fields in the process of mixture formation in HCCI mode are shown in Fig.5. Injection begins from 82 °CA BTDC with its duration of 25 °CA. At 15 °CA after the start of injection, the fuel injection develops and already near the piston top side. In the middle and front parts of fuel injection, the fuel mole fraction is about 0.15 and its temperature is near 450K, as Fig.5(a) shown. In addition, ten nozzles are divided into two types: each diameter of upper 6 nozzles is 0.25mm, while the below 4 nozzles is 0.18mm. The below 4-sprays are close to the upper 6-sprays. Therefore, the shape of the middle concentration field is rectangle, as Fig.5 shown. The in-cylinder fuel concentration and temperature fields at 25 °CA BTDC are shown in Fig.5(b), when injection has already completed with the rich mixture forming a zone, and the fuel continues mixing. The temperature of the zone is about 700K, where its mole fraction is about 0.05. The first phase reaction takes place slowly near the zone, where its temperature is about 750K, which is determined by its concentration and temperature. Most mixtures are lean, namely, the air equivalence ratio is over 3.5. Furthermore, as the temperature field shown, due to the endothermic fuel vaporization, the temperature of rich homogenous mixtures is lower than the lean homogenous mixtures.



(a) 67 °CA BTDC (b) 25 °CA BTDC

Fig.5 In-cylinder fuel concentration and temperature fields in the mixture formation process under the HCCI mode

According to Fig.5(b), the in-cylinder mixtures are divided into three parts: the air/fuel equivalence ratio at the circular zone is about 0.4, the air/fuel equivalence ratio in the lateral zone is about 1, and the air/fuel equivalence ratio in the center zone is about 3.5. The mixtures are stratified homogeneous.

As the density and temperature field shown, the rich mixtures accumulate in the ω-type combustion chamber. The mixtures near the cylinder wall are somewhat rich and impinging wall while the mixtures in the center of cylinder are too lean to ignite. These result in high unburned HC emissions and low thermal efficiency. Its experimental result is 18.66%. With the piston moving up, the mixtures are more homogeneous and multispot burning (this is HCCI combustion). The experiment shows that the value of NO_x and smoke emissions is zero. However, the combustion system must be changed in order to avoid fuel impinging the cylinder wall.

VI. Conclusion

This paper evaluates CO, HC, NO_x and smoke emissions and thermal efficiencies of a two-stroke Diesel engine at a given operating condition in two combustion modes, and explains the experimental results by numerical simulations of mixture formation successfully. The normal combustion mode of Diesel engine is the diffusion combustion, namely "fire containing fuel" form. This combustion mode results in the formation of NO_x and smoke. However, it has high average temperature in the cylinder, which is helpful to decrease CO and HC emissions. Diesel HCCI combustion is a premixed combustion mode by homogeneous mixture before combustion, which reduces the emissions of NO_x and smoke, but high CO and HC emissions due to its low average temperature.

Future work on this research is highly promising. HCCI combustion is actualized by early-injection, which results in high unburned fuel emissions and relatively low thermal efficiency due to using its original combustion system. Therefore, comparing numerical simulation, some works should be done for more satisfied thermal efficiency and lower HC and CO emissions, such as machining new combustion system, etc.

References

[1] S. Onishi, S. H. Jo, K. Shoda, P. D. Jo, S. Kato, "Active thermo-atmosphere combustion (ATAC) - a new combustion process for internal combustion engines," SAE Paper 790501, 1979.

[2] R. H. Thring, "Homogenous charge compression ignition (HCCI) engine," SAE Paper 892068, 1989.

[3] H. S. Rudolf, E. R. Charles, "Homogeneous charge compression ignition (HCCI): benefits, compromises, and future engine applications," SAE Paper 1999-01-3682, 1999.

[4] U.S. Department of Energy, "Homogeneous charge compression ignition (HCCI) technology - a report to the U.S. Congress," April 2001.

[5] T. J. Lin, W. H. Su, Y. Q. Pei, "Study of auto-ignition and burning rate control on the process of Diesel engine HCCI combustion," *Natural Science Progress*, vol. 5, pp. 518–522, May 2003.

[6] X. C. Lu, L. B. Ji, J. J. Ma, H. Zhen, "Combustion stabilities and cycle-by-cycle variations of n-heptane homogenous charge compression ignition combustion," *Energy & Fuels*, vol. 21, pp.1468-1473, May 2007.

[7] C. Takemi, A. Takashi, "In-cylinder control of smoke and NOx by high-turbulent two-stage combustion in Diesel engines," SAE Paper 962113, 1996.

[8] C. A. Alex, "Combustion advancements in gasoline engines," *Energy Conversion & Management*, vol. 48, pp. 2751-2761, Nov. 2007.

[9] M. A. Salvador, L. F. Daniel, K.W. Charles, J. R. Smith, P. William, D. Robert, C. Magnus, J. Bengt, "A multi-zone model for prediction of HCCI combustion and emissions," SAE Paper 2000-01-0327, 2000.

[10] L. E. William, A. Apoorva, A. L. George, "Modeling of HCCI combustion and emissions using detailed chemistry," SAE Paper 2001-01-1029, 2001.

[11] S. C. Kong, R. D. Reitz, "Use of detailed chemical kinetics to study HCCI engine combustion with consideration of turbulent mixing effects," *Journal of Engineering for Gas Turbines and Power*, vol. 124, pp. 702-706, July 2002.

[12] S. Mosbach, H. Su, M. Kraft, A. Bhave, F. Mauss, Z. Wang, J. X. Wang, "Dual injection homogeneous charge compression ignition engine simulation using a stochastic reactor model," *International Journal of Engine Research*, vol. 8, pp. 41-50, Jan. 2007.

[13] V. I. Golovitchev, N. Nordin, R. Jarnicki, J. Chomiak, "3-D diesel spray simulations using a new detailed chemistry turbulent combustion model," SAE Paper 2000-01-1891, 2000.

[14] L. A. Vulis, "Thermal regimes of combustion," McGraw-Hill Book Company, Inc, New York, 1961.

[15] Z. L.Zheng, M. F. Yao, "Numerical study on the chemical reaction kinetics of n-heptane for HCCI combustion process," *Transactions of CSICE*, vol. 22, pp. 227-234, June 2004.

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