Optimizing Hydrogen and Ammonia Injection Timing for Enhanced Mixture Formation in Internal Combustion Engines

ABSTRACT

Hydrogen and ammonia are two carbon-free alternative fuels for engines. They represent some of the most viable pathways toward achieving our objectives of energy conservation and reducing emissions. To research the quality of the hydrogen-ammonia-air mixture formation under different hydrogen/ammonia injection timing, a three-dimensional simulation model for a PFI(Port Fuel Injection)hydrogen internal combustion engine with the inlet, outlet, valves and cylinder was established using Converge software. Research focused on the space distribution characteristics and variation law of velocity field, concentration field and turbulent kinetic energy under different injection timings in order to reveal the influence of these parameters on hydrogen-ammonia-air mixture formation process. The results showed that hydrogen injection should be neither too early nor too late. Backfiring can be initiated too early or too late. Therefore, the optimum starting point for hydrogen/ammonia injection should be 338°CA.

Keywords:Hydrogen; ammonia; Mixture distribution, injection timing.

1. INTRODUCTION

In recent years, the problem of global warming caused by carbon dioxide emissions from the burning of fossil fuels has attracted considerable attention from all sectors of society, and global carbon dioxide emissions have been increasing year on year, with the burning and use of fossil fuels still accounting for a large proportion of total carbon emissions. Increasingly stringent emission regulations and the national policy direction of green and clean energy consumption have advanced the new trend of green and renewable new energy development, making the development of clean energy occupy an important position in the automotive field[1]. And hydrogen/ammonia has outstanding advantages among many alternative fuels due to its unique physical and chemical properties[2,3].

Hydrogen stands out as the most promising fuel due to its array of favorable characteristics, including its high heating value, rapid flame propagation rate, and notable reaction activity[4,5]. Benbellilconducted experiments on a dual-fuel compression-ignition engine, finding that blending natural gas with hydrogen improved combustion, reduced HC and CO emissions, but cautioned against H2 concentrations exceeding 50% at high loads due to engine knock[6]. Gu evaluated the combustion and emission performance of the ammonia hydrogen mixed fuel engine. With the hydrogen mixing ratio increasing, the flame propagation speed increasing, the peak of heat release rate increasing, and the ignition timing advance[7]. Frigo investigated the performance impact of burning ammonia/hydrogen dual fuel on a four-stroke gasoline engine, noting that the load primarily influences the ammonia-to-hydrogen ratio, with ignition and combustion rates improving after adding hydrogen, albeit with slightly reduced performance compared to gasoline combustion[8].

Wang studied the performance effects of a diesel-fueled ammonia-hydrogen hybrid engine on a high-pressure common rail compression ignition engine, revealing substantial improvements in power and economy with the addition of hydrogen fuel, while noting increased NOx emissions but significant reduction in N2O emissions beneficial for global warming mitigation[9].

Pure ammonia combustion in engines poses challenges due to high boundary conditions for combustion and prolonged initial flame development[10]. Dimitriouresearch discovered that achieving pure ammonia combustion is challenging due to its higher ignition temperature compared to diesel, necessitating initial diesel ignition in diesel engines; however, slow flame propagation and high vaporization latent heat values hinder complete combustion, leading to ammonia escape in cases of excessive ammonia blending[11]. Common solutions involve blending combustion with carbon-containing fuels (natural gas, methanol, diesel, gasoline) and hydrogen to lower combustion boundary conditions[12,13]. Sechul~~i~~ investigated a natural gas/ammonia dual-fuel ignition engine, replacing over 50% of natural gas with ammonia fuel, resulting in a more than 28% decrease in CO2 emissions, alongside a reduction in laminar flame propagation speed as ammonia fuel proportion increased[14]. Grannell explored the combustion characteristics of ammonia/gasoline under stoichiometric conditions, and they found that there were no fixed blending ratios between ammonia and gasoline suitable for all operating conditions[15]. Sahin et al. studied the impact of co-combusting an ammonia solution (25% ammonia + 75% water) with diesel fuel on a small diesel engine, finding that while adding ammonia solution to the intake manifold enhanced engine efficiency, it worsened emissions, increasing CO, HC, and NOx concentrations in the exhaust gas, with only CO2 emissions decreasing as the ammonia share increased[16].

Combining ammonia and hydrogen supply modes offers flexible fuel synergy control strategies to enhance engine performance in internal combustion engines. Rocha numerically examined premixed flame propagation and NOx emissions in ammonia/hydrogen mixed fuel, finding that while hydrogen addition accelerates flame speed, it significantly increases NOx emissions[17]. Ichikawa investigated laminar combustion rate and Markstein length in premixed combustion of ammonia-hydrogen mixtures, concluding that using hydrogen as a combustion promoter enhances power and stability, with an optimal hydrogen proportion exceeding 20%[18].

In summary, most research on ammonia-hydrogen engines has concentrated on port injection, which, while convenient, reduces volumetric efficiency and power density due to H2 crowding in the cylinder during the intake stroke. This inspired the present study to investigate the fuel trapping ratio at different injection timings and the velocity and turbulence fields within the cylinder under different injection timings. The research results can promote the practical application of hydrogen fuel in internal combustion engines by providing valuable insights into optimizing combustion processes and enhancing engine efficiency. This could lead to the development of more sustainable and environmentally friendly transportation solutions, contributing to the transition towards cleaner energy sources and reducing carbon emissions in the automotive sector.

2. COMPUTATIONAL MODEL AND RESEARCH PROGRAM

2.1 Geometric model

In this paper, a complete closed geometry model consists of inlet and exhaust port, valves and cylinder is established using the three-dimensional modeling software SolidWorks, as shown in Fig. 1(a). The basic parameters of the prototype are shown in Table1. In order to systematically study the flow and combustion process of the mixture in-cylinder of a PFI hydrogen internal combustion engine, the initial and boundary conditions (including components, temperature, pressure, etc.) were set according to the actual working process of the internal combustion engine with the upper stopping point at the end of the compression stroke as 0 °CA. The base mesh size is 4 mm, with Adaptive Mesh Refinement

(AMR) implemented in high-velocity and high-temperature curvature areas.**The engine test bench is shown in Fig. 1 (b).**

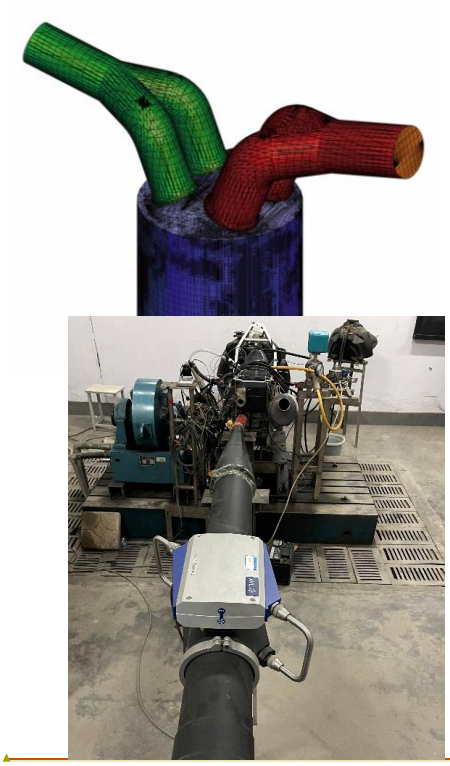

Fig. 1.(a)3D Engine Model(b) Engine test bench

Table 1. Parameters of the PFI hydrogen ICE prototype studied in this subject.

Parameters	Indexes
Connecting rod length/mm	160
Cylinder diameter/mm	94
Stroke/mm	85
Compression ratio	9.7:1
Maximum power/kW	30
Maximum power speed/r/min	6000
Maximum torque/N m	51
Maximum torque speed/r/min	4500

2.2Numerical model

The CONVERGE software is a computational fluid dynamics software that allows the simulation of combustion, emissions, etc. The main sets of control equations are the mass conservation equation, the momentum conservation equation and the energy conservation

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equation. In this paper, CONVERGE software is used to establish a 3D simulation model for simulation research. The sub models used in modeling are as follows:
Turbulence model: The RNG k-ε turbulence model was chosen, which has a high accuracy of eddy calculation and can better predict the effects of transient flows with a wider range of applications; Spray model: CONVERGE software accurately models fuel atomization, evaporation, crushing, and collision using the KH-RT spray fragmentation model, NTC collision model, and wall film model for droplet-wall interaction; Combustion model: To ensure the accuracy of the simulation study and better simulate the ignition process and combustion process in the cylinder, the SAGE combustion model couples the n-Heptane/hydrogen/ ammonia reaction mechanism in the simulation study.
Mass conservation equation:

$$\frac{\partial \rho}{\partial t}+\frac{\partial \rho u_i}{\partial x_i}=S \tag{1}$$

where: t is time; "ρ" is the fluid density; u is the velocity vector; and S is the source term, originating from evaporation or other submodels.
Equation of conservation of momentum:

$$\frac{\partial \rho u_i}{\partial t}+\frac{\partial \rho u_i u_j}{\partial x_j}=-\frac{\partial P}{\partial x_i}+\frac{\partial \sigma_{ij}}{\partial x_j}+S_i \tag{2}$$

$$\sigma_{ij}=\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)+\left(\mu^{'}-\frac{2}{3}\mu\right)\left(\frac{\partial u_k}{\partial x_k}\delta_{ij}\right) \tag{3}$$

where: t is time; "ρ" is the fluid density; u is the velocity vector; S is the source term, originating from evaporation or other sub-models; σ_{ij} is the pressure tensor; P is the indicated pressure; μ is the viscosity; $\mu^{'}$ is the expansion viscosity, which has a value of 0; and δ_{ij} is the Kronecker function.
Energy conservation equation:

$$\frac{\partial \rho e}{\partial t}+\frac{\partial u_j \rho e}{\partial x_j}=-P\frac{\partial u_j}{\partial x_j}+\sigma_{ij}\frac{\partial u_i}{\partial x_j}+\frac{\partial}{\partial x_j}\left(K\frac{\partial T}{\partial x_j}\right)+\frac{\partial}{\partial x_j}\left(\rho D\sum_m h_m\frac{\rho \gamma_m}{\partial x_j}\right)+S \tag{4}$$

where: t is time; "ρ" is the fluid density; u is the velocity vector; S is the source term, originating from evaporation or other sub-models; T is the temperature; γ_m is the mass fraction of species m; D is the mass diffusion coefficient; e is the specific internal energy; K is the coefficient of transport of matter; and h_m is the enthalpy of species m.

2.3 Boundary conditions and initial conditions

In the boundary condition settings for the PFI hydrogen-fueled internal combustion engine, the air inlet boundary is set to the "inlet" pressure parameter type and the exhaust outlet boundary to the "outlet" pressure parameter type. In the boundary condition setting of PFI hydrogen fuel internal combustion engine, the air inlet boundary is set as "inlet" pressure parameter type, and the exhaust outlet boundary is set as "outlet" pressure parameter type. The other wall boundaries are set as "fixed wall" with constant temperature; the inlet valve, exhaust valve and piston are set as "moving wall". Based on preliminary tests and experience, the following boundary conditions have been established as shown in Table 2.

Table 2. Boundary condition setting of PFI hydrogen engine.

Border areas	Boundary type	Setpoint
Air inlet	Inlet	0.1Mpa
Exhaust outlet	Outlet	0.106Mpa
Inlet pipe	Stationary wall	300K
Exhaustpipe	Stationary wall	600K
Inlet valve	Moving wall	550K
Exhaust valve	Moving wall	800K
Cylinder wall	Stationary wall	480K
Pistons	Moving wall	600K
Cylinder head	Stationary wall	600K

2.4Model validation

Fig. 2illustrates the impact of base grid size on in-cylinder pressure, showing minor differences when the size is below 4.0 mm, thus justifying a 4 mm base grid size for simulation accuracy and efficiency.

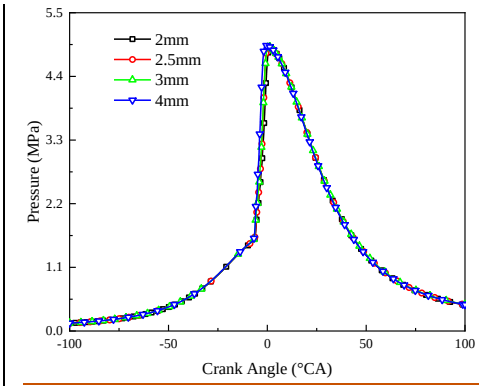

Fig.2.The effect of base grid size on in-cylinder pressure.

Fig. 3 shows the comparison curves of the test and simulated in-cylinder combustion pressures of the hydrogen combustion engine under the same working conditions. It can be seen from Fig. 3 that the experimental and simulation results are in good agreement, and the maximum error is less than 5%. Therefore, it can be proved that the selected hydrogen internal combustion engine model can be used to simulate the in-cylinder combustion process, and the simulation results obtained are highly accurate.

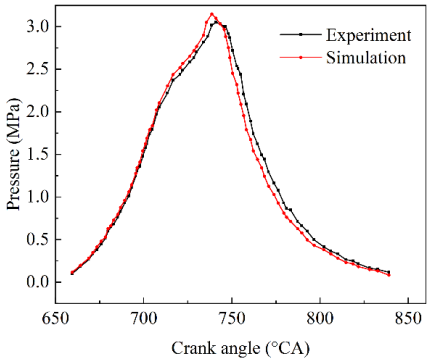

Fig.3.In-cylinder pressure verification.

2.5 Methodology

The experimental programme with different hydrogen/ammonia injection timing with four sets of hydrogen/ammonia injection timing consists of the following: H338-N338, H338-N349, H349-N338, H349-N349. Where 'H','N' denotes hydrogen/ammonia and '338','349' denotes injection timing of 338° CA BTDC and 349° CA BTDC.

An operating cycle of an internal combustion engine consists of four processes: intake, compression, work and exhaust, of which the intake process directly determines the quality of the formation of the mixed fuel and air and has an important influence on the subsequent combustion and emission processes in-cylinder. Hydrogen injection timing is an important factor in controlling the quality of hydrogen-air mixture formation, which directly influences the development and spatial-temporal distribution of hydrogen in the intake tract and into the cylinder, thus essentially inhibiting the problem of intake tract clogging in PFI hydrogen combustion engines. Selecting the optimum timing for hydrogen injection is critical to maximising performance and minimising problems such as intake tract plugging and abnormal combustion. The engine speed is 1800 rpm, the equivalence ratio is 1 and the orifice diameter is 5 mm. Fig. 4 shows the comparison between the set injection volume and the in-cylinder fuel mass at different injection timings with the intake valve closed. From the table, it is learnt that when the injection timing is 338°CA BTDC and 349°CA BTDC, the injection efficiency is the highest and the in-cylinder fuel quality meets the requirements, so the injection timing of 338°CA BTDC and 349°CA BTDC is used as the basis for the next study.

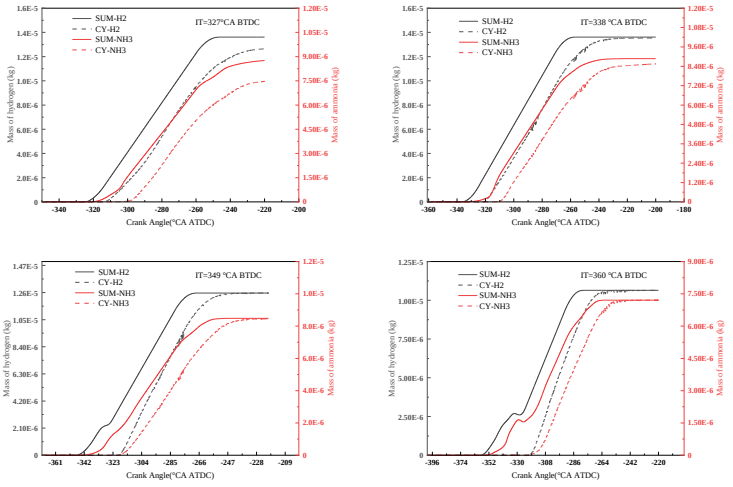

Fig.4.In-cylinder fuel capture at different IT.

3. RESULTS AND DISCUSSION

3.1 Effect of injection timing on air flow in the intake pipe

Figure 5 shows the variation of inlet charge mass flow rate with engine crankshaft angle corresponding to five injection timings: H338-N338, H338-N349, H349-N338, H349-N349. In Fig. 5, the vertical coordinate represents the charge inlet mass flow rate, with negative values characterising normal charge flow into the inlet and positive values characterising abnormal charge backflow out of the inlet, representing the occurrence of intake blockage. The increases and decreases described below are based on the zero tick mark, and the increases and decreases are compared in absolute magnitude.

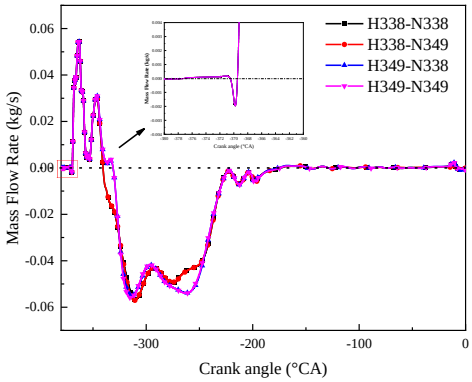

Fig.5.Variation of air mass flow with crankshaft under different IT

The results in Fig. 5 show that for different injection timing, when the air inlet is opened, the inlet mass flow rate increases slightly in the direction of the inflow inlet and then starts to increase in the direction of the outflow inlet and crosses the zero tick mark, increases rapidly to a peak and then returns to close to the zero tick mark, and then increases again in the direction of the outflow inlet to a peak before returning to the negative range. This is due to the initial period of intake, the valve lift is low, the charge into the intake pipe is hindered, filling the intake pipe after the intake pipe backflow phenomenon occurs, with the gradual opening of the intake valve, the backflow phenomenon is weakened. After the start of the injection timing, due to the small molecular weight of hydrogen, hydrogen is rapidly expanded after being injected into the intake tract, resulting in a rapid increase of the intake mass flow along the outflow direction of the intake tract, and air is rapidly expanded by the hydrogen and forced out of the intake tract, i.e. the air in the intake tract is a backflow phenomenon. This phenomenon is referred to as inlet air blocking phenomenon. At the end of hydrogen injection, there is no more hydrogen expansion and as the piston moves downwards, hydrogen/ammonia is pushed into the cylinder by the air and the air obstruction by hydrogen is reduced and the charge in the intake tract is always in the inflow direction and there is no intake tract backflow. When the hydrogen injection timing was earlier (338° CA BTDC), the intake tract blockage was relieved relatively early, which was more conducive to mixing fuel and air in the cylinder.

3.2Effect of Injection Timing on Velocity Field

Varying the timing of hydrogen injection is of great importance to the law of variation of the in-cylinder velocity field in hydrogen engines. By analysing the velocity field, it is possible to gain insight into the flow characteristics of hydrogen in the combustion chamber, thus optimising the combustion process and improving engine efficiency and performance.

As can be seen from the figure, in-cylinder mixture at the beginning of the pressure under the action of the rapid flow to the cylinder. Following an impediment encountered at the intake valve, the amalgamated mixture navigates through a circular conduit between the intake valve and the cylinder head, ultimately coalescing into a localized region of heightened velocity proximal to the intake valve seat. At this juncture, the confined space within the cylinder constrains the voluminous influx, prompting the high-velocity mixture to collide with the cylinder head and piston crown, thereby engendering a pair of counter-rotating vortices under the influence of geometric boundaries.

As the intake valve opening continues to increase, the mixture fills the in-cylinder space at a higher flow rate under the effect of injection push and space expansion, and the fuel and air are further mixed. After the piston reaches the lower stop, the in-cylinder space reaches its maximum and the overall flow rate of the mixture slows down. As the compression stroke begins and the piston travels upward, the high flow velocity of the mixture gradually dissipates, with the high flow velocity area existing only at the top of the piston, and the velocity field in other areas being nearly uniformly distributed at an overall velocity. At the moment of ignition, the mixture velocity in-cylinder converges and the velocity field is uniformly distributed.

Longitudinal comparison shows that the velocity field of the mixture in the cylinder does not change significantly at the beginning of the intake period, and that, overall, areas of high flow velocity are formed around the valves. Before the piston moves to the lower stop, as the injection timing is delayed, the area of the high-speed area in the cylinder decreases, which is not conducive to rapid mixing of air and fuel; At the beginning of the compression stroke, the high-speed mixture in the cylinder is gradually distributed to the right side of the piston and the left side of the cylinder wall, and the whole tends to be more homogeneous; when the piston moves to the upper stop, the timing of the hydrogen/ammonia injection is all for the -330° CA conditions, with a more uniform distribution of the velocity field.

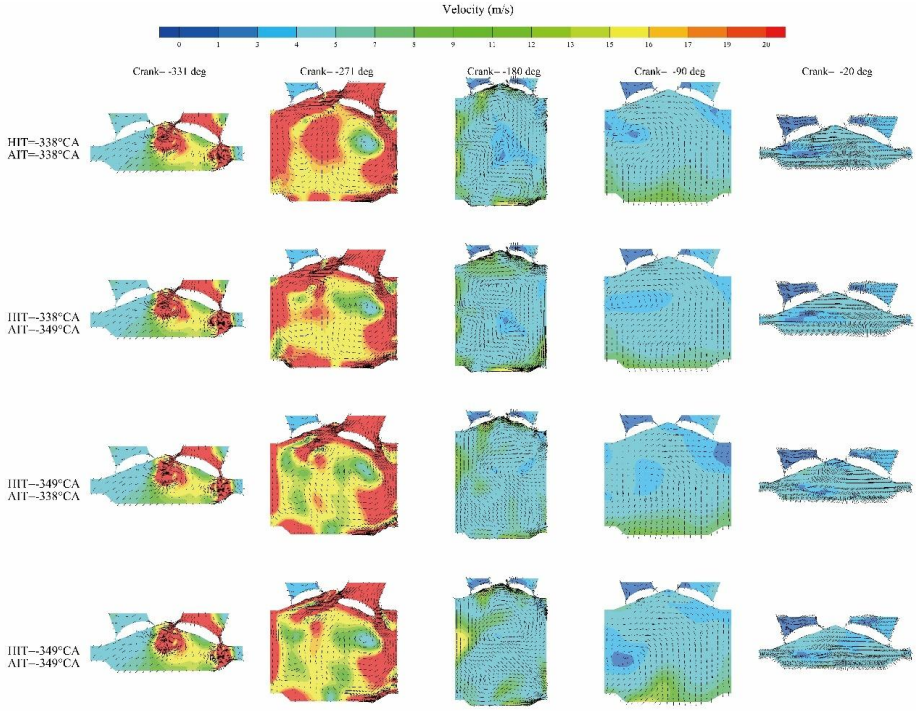

Fig. 6. The development process of the velocity field

3.3Effect of Injection Timing on TKE

In practical operation, the port fuel injection (PFI) hydrogen internal combustion engine constantly undergoes a turbulent and highly disordered motion within the confines of its cylinder. Such a phenomenon exerts a discernible influence on the spatio-temporal distribution of various components and the dynamics of both the air-fuel mixture and the flame propagation, thereby exerting a formidable influence on the quality of mixture formation, combustion processes and emission characteristics.

As shown in Fig. 7, at the very beginning of the intake stroke, the high flow rate of the mixture enters the combustion chamber through the valves, and high intensity turbulence is formed around the intake valves, which corresponds to the large scale vortex clusters in the velocity field. As the piston moves down and the intake valve opens, a large amount of gas enters the cylinder along the intake valve and cylinder wall, with higher turbulent kinetic energy at the centre of the cylinder guided by the wall. Towards the end of the inlet stroke, the high turbulent kinetic energy mixture dissipates into low-intensity turbulence, thus favouring homogeneous mixing of the mixture. During the compression stroke, the turbulent kinetic energy enhanced by the compression stress and the shear force between the gas and the wall is not enough to compensate for the rapid dissipation of the turbulent vortices. At this point, the average turbulent kinetic energy in-cylinder continues to decrease. With the upward movement of the piston, the large-scale turbulent vortices continue to break up into small-scale turbulent vortices, and the turbulent motion in-cylinder gradually develops to be

dominated by the small-scale turbulent vortices, and the turbulent kinetic energy can be enhanced accordingly.

A comprehensive comparison shows that the initial high turbulence kinetic energy area is larger when the injection timing is advanced. The advance in injection timing results in the mixture entering the cylinder earlier, which encourages a more even distribution of the mixture in-cylinder. This advance in injection results in better mixing of the mixed fuel with the air in-cylinder, ensuring that the fuel and oxygen are in full contact to form a more homogeneous mixture. As a result, at the moment of ignition, the fuel can be burned more quickly and fully, thus improving combustion efficiency and combustion performance. In addition, injection timing advance also helps to reduce the stagnation time of the mixture in-cylinder, reducing incomplete combustion and emissions.

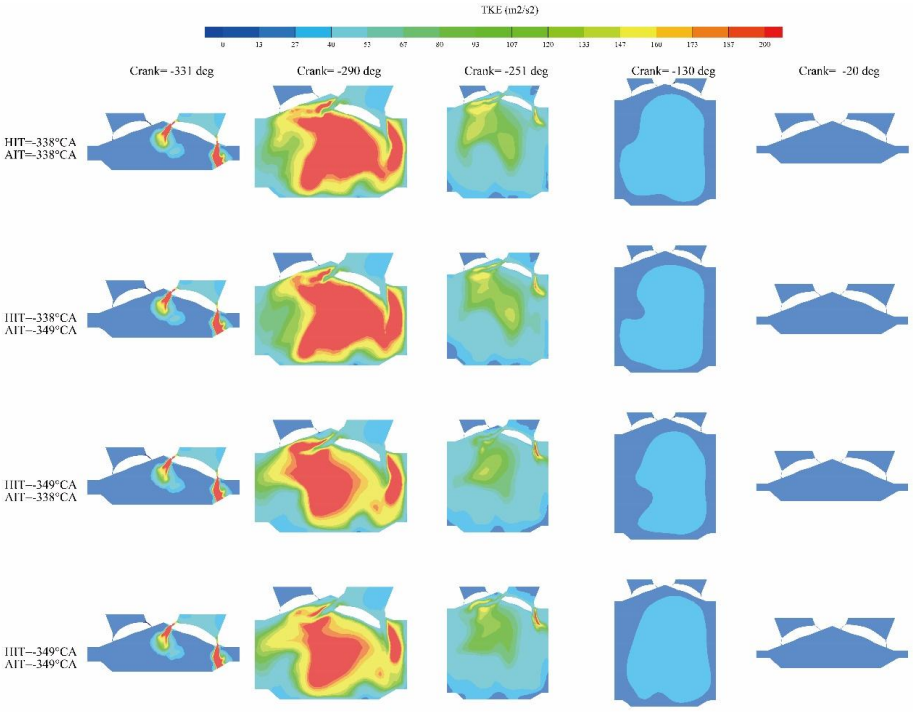

Fig. 7. Changes of turbulent kinetic energy in the cylinder

4. CONCLUSION

By studying the spatial distribution characteristics and change laws of total hydrogen quality inside and outside the cylinder, velocity field and turbulent kinetic energy of hydrogen internal combustion engine under different injection timings in the intake pipe, the influence of these parameters on the hydrogen-ammonia-air mixture formation process is revealed. The main findings are shown below.

To improve the uniformity of the gas mixture, the hydrogen injection should be neither too early nor too late. the relative residence time of the high concentration gas mixture in the

intake is longer if the injection is too early, which easily leads to backfire. If the hydrogen injection is late, the increase in cylinder pressure hinders the process of the hydrogen entering the cylinder. This also increases the dwell time of the hydrogen at the intake valve. At this point, the mixture will be less uniform. If the hydrogen injection is delayed, the residual hydrogen in the intake pipe can also increase, which increases the possibility of backfire. Therefore, in a comprehensive consideration, the optimum starting point for hydrogen/ammonia injection should be 338°CA.

Future areas of research will include further optimisation of injection timing, considering sequential hydrogen/ammonia injection or multiple injection.

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COMPETING INTERESTS

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

AUTHORS' CONTRIBUTIONS

Shuman Guo: Conceptualization, Methodology, Validation, Formal analysis, Writing-original draft, Writing – review & editing. **Zhichao Lou**: Software, Investigation, Formal analysis, Writing - original draft.**Xu Zhang**: Software, Formal analysis.**Shaokai Shen**: Investigation, Software, Formal analysis. **Jintao Meng**: Data curation.**Jiaqi Wang**: Data curation.**Chunjian Zhou**: curation.

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