

CHEMICAL KINETIC ANALYSIS OF IN-CYLINDER ION CURRENT GENERATION UNDER DIRECT WATER INJECTION WITHIN INTERNAL COMBUSTION RANKINE CYCLE ENGINE

by

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Direct water injection provides feasible solution for combustion optimization and efficiency enhancement within internal combustion Rankine cycle engine, while the feedback signal of close-loop direct water injection control is still absent. Ion current detection monitors in-cylinder electron variation which shows potential in revealing direct water injection process. For better understanding of unprecedented augment of ion current signal under direct water injection within internal combustion Rankine cycle engine, a chemical kinetic model is established to calculate the effect of intake oxygen fraction, fuel quantity, initial temperature, and residual water vapor on in-cylinder electron formation based on GRI Mech 3.0 and ion current skeleton mechanism. The simulation results indicate direct water injection process show significant impact on in-cylinder electron formation through chemical interactions between H₂O and other intermediate species including HO₂, O₂, CH₃, and H, these reactions provides additional OH radical for propane oxidation facilitation, which result in large portion of CH radical formation and therefore, lead to higher in-cylinder electron generation. The initial temperature plays a vital role in determining whether residual water vapor show positive or negative effect by in-cylinder temperature co-ordination of direct water injection. Results of this work can be used to explain phenomenon related to direct water injection and ion current signal variation under both internal combustion Rankine cycle or traditional petrol engine.

Key words: chemical kinetic, ion current, internal combustion Rankine cycle, water injection

Introduction

The internal combustion engine (ICE) is facing severe challenges in modern automotive powertrains industry as fuel consumption and emissions regulations become more and more stringent. Compare with the battery electric vehicle and fuel cell vehicle (FCV), the main obstacles of ICE are relatively low tank-to-wheel efficiency and in-use emissions [1, 2]. While the brake thermal efficiency (BTE) of modern commercial petrol ICE has improved signifi-

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cantly by implementation of advanced engine optimization technologies including lean/diluent combustion [3], Atkinson/Miller cycle [4], intensive in-cylinder tumble flow [5], variable compression ratio [6], controllable auto-ignition [7], *etc.*, the overall TTW efficiency remains under 45% [8]. The requirement for novel combustion concept which is capable in realizing extreme high thermal efficiency while achieving zero emission is becoming more and more urgent. As the researchers and scholars continual present novel ICE combustion concepts, the internal combustion Rankine cycle (ICRC) seems to be one the most promising solutions [9].

Inspired by oxy-fuel combustion utilized in advanced zero emission power plant [10, 11], the ICRC concept is proposed by Bilger in [12], and its feasibility in transplanting this concept into automotive ICE is further verified by co-operating with the authors [13], as shown in fig. 1. The air intake is replaced with O_2/CO_2 mixture, by doing so, the NO_x emissions can be fully avoided. Theoretically, there are only CO_2 and steam within the exhaust gases, meanwhile, the CO_2 and steam is further separated through condensation, the acquired water is recycled and pressurized into high pressure water, the harvested high pressure water acts as heat absorption agent which in turns heat up to around 433 K, the high temperature and pressure water is then directly injected into combustion chamber at specific timing during combustion process to optimize in-cylinder oxy-fuel combustion which controls the in-cylinder temperature as needed, on the other hand, the injected water evaporate into high temperature and pressure steam rapidly, the generated steam acts as additional working fluid,

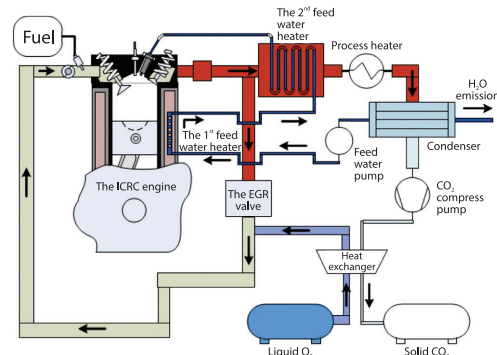


Figure 1. Schematic diagram of ICRC concept [14]

provide extra work as the piston moves downward, this combination effect of direct water injection (DWI) within ICRC concept proved stable combustion and high efficiency. Meanwhile, the separated CO_2 further exchange heat in another heat exchanger with liquid O_2 which solidified CO_2 into dry ice, the liquid O_2 transforms into gaseous O_2 and utilized as the oxidizer, the dry ice is stored in gas cylinders and recycles as the vehicle arrived at certain locations, by doing so, the CO_2 emission within tradition ICE can be eliminated. As calculated by the authors, the ICRC concept obtains similar efficiency compare of FCV while achieve zero emission during vehicle operation [14].

As the proposal of ICRC concept, the authors have conducted comprehensive studies completing ICRC theory and establishing prototype engines. A more comprehensive 0-D theoretical cycle is proposed by utilization of instant in-cylinder water evaporation assumption [14] based on Otto cycle, the effect of engine operation and DWI parameters including revolution, load, intake pressure, water injection mass, water injection pressure, and water injection temperature on ICRC efficiency were investigated numerically, the water injection temperature, water injection mass and engine load were proved to be the dominant parameters for the cycle efficiency enhancement [15]. Meanwhile, the water injection temperature and water injection mass are limited by exhaust temperature and exhaust mass-flow rate, as they provide energy for heating up the injection water, by considering the limitation of exhaust energy, the optimum thermal efficiency boundary of ICRC concept is confirmed, an optimum 62% thermal efficiency is acquired [16].

Besides the aforementioned theoretical studies, the authors also conducted experimental verifications by establishing ICRC prototype engines. The first generation of ICRC prototype engine is constructed based on the modification of motorcycle engine with high revolution and small bore, the compression ratio is fixed at 9.2:1 [17], the second generation of ICRC prototype engine is modified from a Diesel engine with variable compression ratio from 9.5:1 to 17:1 [18]. The key subsystems such as O_2/CO_2 intake system and direct high temperature water injection system are developed by authors to fulfill the requirements as ICRC engine operated, the O_2/CO_2 intake system provide variable OF from 21-100% and direct high temperature water injection system provide water injection pressure varies from 15-35 MPa while water injection temperature varies from 298-473 K under consecutive cycles [19]. The experimental results indicated that the spark ignited (SI) ICRC engine can be operated under intake oxygen fraction (OF) 21-60%, as the increment of intake OF lead to lifted in-cylinder pressure rise rate and intensive abnormal combustion, the feasibility of utilizing in-cylinder water injection mitigate abnormal combustion is also investigated [20]. Meanwhile, the prototype engine efficiency is proved to be enhanced as water injection mass and temperature increased, the mechanism of cycle efficiency lies in the generation of high temperature and high pressure steam during in-cylinder water evaporation, therefore, improvement of in-cylinder temperature (*e.g.* optimized engine load) lead to faster in-cylinder water evaporation, which provide larger increment in cycle efficiency optimization [21]. Although the DWI show huge potential in reducing abnormal combustion, the elimination of abnormal combustion is still a huge problem, therefore, within SI ICRC engine, large portion of exhaust gas re-circulation (EGR) is needed for lowering in-cylinder temperature [22], the utilization of EGR limited the potential of ICRC concept as it shows negative impact on cycle efficiency optimization. In order to solve this problem, the compression ignition (CI) combustion mode is tested within the second generation of ICRC prototype engine, by utilization of homogeneous and heterogeneous charge CI, a significant reduction of EGR utilization is realized, intake OF under homogeneous charge compression ignition (HCCI) varies from 70-100% [23], while OF decreased to 65-75% under traditional diffusion flame CI [24]. Within the CI ICRC, the experimental and 3-D simulation results indicated that the enhancement of DWI also lead to increment in cycle efficiency, and thanks to the high compression ratio under CI ICRC operation, the BTE is significantly improved to 46.6% [25].

As introduced previously, the DWI is a key control method of in-cylinder combustion optimization and cycle efficiency enhancement within ICRC concept, but the feedback signal of in-cylinder water injection process is absent. To fill in this gap and improve DWI control process, the author proposed to utilize ion current detection within ICRC concept as the in-cylinder combustion status directly affect ion current generation [26]. As presented in the experimental results, the DWI show huge impact on in-cylinder ion current signal which indicate that ion current signal show potential in monitoring in-cylinder water injection process. In [26], the amplitude of ion current signal increased as DWI activated, it is concluded that the trapped in-cylinder steam residual contributes to the enhancement of ion current signal but the chemical kinetic analysis remains to be clarified. This work established a simplified constant closed chamber model to investigate the chemical kinetic of propane premixed combustion with or without DWI based on in-cylinder ion skeleton mechanism [27], which provided fundamental information about ion current signal variation during DWI process.

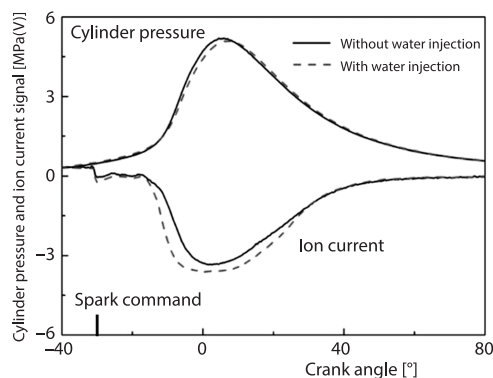


Figure 2. Comparison between water cycle and dry cycle [26]

Computational model

As presented in previous studies [26], the characteristics of ion current signal under water injection is significantly altered. As illustrated in fig. 2, the amplitude of detected ion current is increased with its phase advanced, it is explained by using residual water vapor within the next cycle after water injection, this conclusion is drawn as the characteristics of ion current signal restored as water injection deactivated for few cycles, as shown in fig. 3(a), and the beginning of alteration in ion current signal can only be discovered in the next cycle after water injection involved, as shown in fig. 3(b).

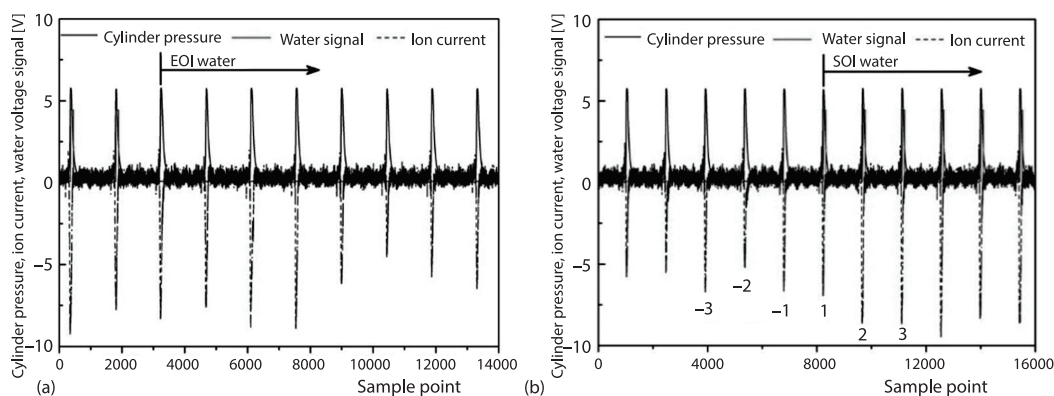


Figure 3. Ion current signal during cycle transition; (a) water to dry cycle and (b) dry to water cycle [26]

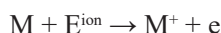
Although the explanation seems reasonable, the direct evidence of water steam enhancement in ion current signal alteration is still absent, in order to provide fundamental mechanism of interaction between in-cylinder residual water vapor and ion generation, the chemical kinetic investigation is conducted by utilizing Chemkin-Pro. During the establishment the computational model, it is noted that the combustion process of ICRC prototype engine is extremely complicated, the involvement of oxy-fuel combustion, EGR, and most importantly, water injection is quite difficult to simulate within 0-D chemical kinetic analysis. To be more specific, the DWI within ICRC engine involves complicated physical process (such as mixing, evaporation, etc.) and chemical process (such as water vapor decomposition, interaction with hydrocarbon fuel, etc.). As the DWI control strategies mainly injected high temperature and pressure water around firing top dead center (fTDC), to simplify the simulation boundary conditions, closed homogeneous batch reactor is utilized to simulate the combustion chamber around fTDC, different fractions of residual water vapor are introduced during model initiation, the fractions of propane, oxygen, CO_2 are carefully selected as it is utilized in the experiments. The initial pressure is selected as the maximum in-cylinder pressure illustrated in fig. 2, and the initial temperature varies from 2000-4000 K to investigate the effect of residual water vapor in ion current generation under different in-cylinder temperatures. The specific simulation boundary conditions are present in tab. 1.

Table 1. Boundary conditions of established computational model

Parameter	Content
Fuel	Propane-C ₃ H ₈
Intake fluids	O ₂ , CO ₂
Oxygen fraction [%]	45~65%
Fuel injection quantity [mg]	45~55
Intake volume [ml]	503
In-cylinder temperature [K]	2000~4000
Residual water quantity [mg]	40~200
In-cylinder pressure [MPa]	5.78

The GRI-Mech 3.0 is selected as the chemical mechanism and thermal dynamic input to calculate the chemical reaction process. The GRI-Mech 3.0 is a well-verified chemical mechanism of methane and related gaseous hydrocarbon fuels which contains 325 reactions and 53 species [28]. More importantly, to calculate the chemical reaction process of ion generation, a skeleton ion current generation mechanism [27] is utilized in this study, this skeleton mechanism is widely used to simulate in-cylinder ion generation in various studies [29, 30], which contains 32 ion reactions and 9 ion species. By combining the GRI-Mech 3.0 with ion current skeleton mechanism, the chemistry and thermal dynamic profiles are well prepared.

To be noted, as described in the skeleton ion current generation mechanism, there are mainly two ways regarding to ion and electron generation, chemical ionization, and thermal ionization. The thermal ionization mainly occurred at relatively high temperature, as the large molecules including NO and particulate matters generate electrons and ionized atoms:



According to the working principle of ICRC engine, the NO is completely eliminated as the N₂ is absent during combustion, meanwhile, propane is a gaseous fuel injected at intake manifold, which provides abundant time for fuel-oxidant mixing, result in an excellent homogeneous mixture, therefore, the generation of particulate matters is negligible. In conclusion, the primary ion current reactions within ICRC is chemical ionization as presented in tab. 2.

Table 2. Primary ion current reactions within ICRC condition

Reaction	A [cm ³ mol ⁻¹ s ⁻¹]	b	E [kJmol ⁻¹]
CH + O ↔ CHO ⁺ + e	$2.5 \cdot 10^{11}$	0	7.118
CHO ⁺ + H ₂ O ↔ H ₃ O ⁺ + e	$1.51 \cdot 10^{15}$	0	0
H ₃ O ⁺ + e ↔ H ₂ O + H	$2.29 \cdot 10^{18}$	-0.5	0

Computational results and discussion

Effect of ICRC engine operation parameters on in-cylinder electron generation

Compare to traditional petrol ICE, the ICRC engine is capable in changing the in-cylinder oxygen content by adjusting the intake OF, the relatively high oxygen content within ICRC engine lead to significantly variation regarding to in-cylinder combustion process. There-

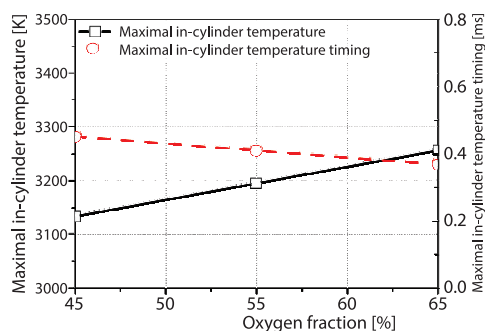


Figure 4. Effect of OF on maximal in-cylinder temperature and its timing

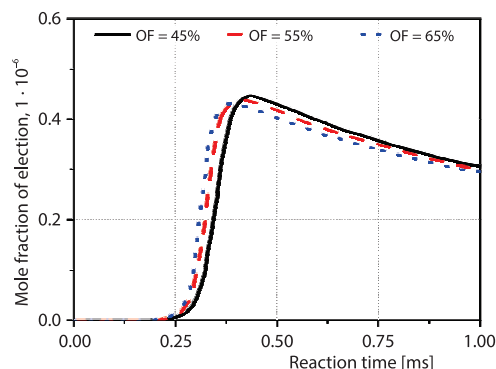


Figure 5. Effect of OF on in-cylinder electron generation

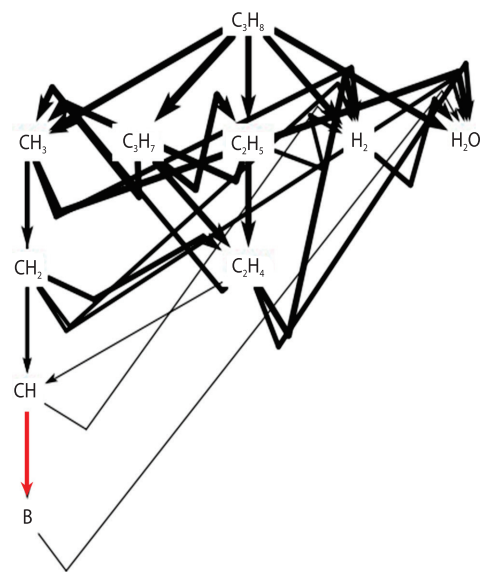


Figure 6. Generation path analysis of electron

fore, it is important to establish a quantitative description of in-cylinder combustion process. As presented in fig. 4, the relationship between maximum in-cylinder temperature and OF is calculated, the increment in OF (from 45%-65%) leads to enhanced in-cylinder temperature (from 3134-3256 K), meanwhile, the maximum in-cylinder temperature timing also advanced as OF increasing (from 0.45-0.37 ms). The aforementioned calculation results are obtained under fuel injection quantity 55 mg and initial temperature 3000 K. This result is in consistent with the experimental results reported in literature [22, 31], which proves that the in-cylinder combustion process is enhanced under elevated intake OF, this phenomenon resulted in providing higher in-cylinder combustion temperature therefore, leads to a quicker steam formation contributes to increment in overall thermal efficiency.

According to the working mechanism of ion current detection technology, the electron generated during combustion is forced to move directly as the in-cylinder high voltage electric field is established, therefore, it is reasonable to evaluate the characteristics of detected ion current signal by calculating the in-cylinder electron formation process. Figure 5 illustrates the mole fraction profile of in-cylinder electron under different intake OF. As it can be seen from the figure, the timing of maximum electron mole fraction is advanced as intake OF increase, which is caused by enhanced propane consumption as oxygen content enriched. Meanwhile, the maximum in-cylinder electron mole fraction under intake OF = 65% is slightly decreased compare to intake OF = 45% which further explanation is needed.

To investigate the decrement of maximum in-cylinder electron generation under elevated intake OF, the reaction path is firstly constructed to clarify which species contribute to in-cylinder electron generation. As presented in fig. 6, the generation path of electron within propane/O₂/CO₂ reaction is acquired at 50% propane consumption rate timing. The propane, as fuel, generates intermediate species includ-

ing CH_3 , C_3H_7 , C_2H_5 , and these species further react and forms CH_2 which lead to an important intermediate specie CH . As described in the ion current skeleton mechanism, CH is the mainly species that forms CHO^+ , which leads to the generation of H_3O^+ and electron. By doing so, it is reasonable to conclude that the variation of in-cylinder electron is largely affected by the generation of CH .

Table 3 presents the effect of OF variation on in-cylinder CH formation. When considering the main reactions of CH formation, $\text{CH} + \text{H}_2 \leftrightarrow \text{H} + \text{CH}_2$ and $\text{OH} + \text{CH}_2 \leftrightarrow \text{CH} + \text{H}_2\text{O}$. These two reactions contribute to the formation of CH in a large content, while their formation rate is significantly reduced as intake OF increased from 45%-65%. Besides, the consumption rate of reaction $\text{CH} + \text{O}_2 \leftrightarrow \text{O} + \text{HCO}$ is relatively enhanced as intake OF increased, which also contribute to the decrement in in-cylinder electron formation as indicated in the data listed in the lower part of tab. 3 (the rate of production of electron generation reaction: $\text{CH} + \text{O} \leftrightarrow \text{CHO} + \text{e}$ is obviously decreased). In conclusion, although the elevated in-cylinder oxygen content leads

Table 3. Effect of OF on in-cylinder CH and electron formation rate

<p>Absolute Rate of Production CH</p> <p> $\text{CH} + \text{O}_2 \leftrightarrow \text{O} + \text{HCO}$ $\text{CH} + \text{H}_2 \leftrightarrow \text{H} + \text{CH}_2$ $\text{OH} + \text{CH}_2 \leftrightarrow \text{CH} + \text{H}_2\text{O}$ $\text{CH} + \text{CO}_2 \leftrightarrow \text{HCO} + \text{CO}$ $\text{CH} + \text{H}_2(+\text{M}) \leftrightarrow \text{CH}_3(+\text{M})$ $\text{H} + \text{CH}_2(\text{S}) \leftrightarrow \text{CH} + \text{H}_2$ $\text{CH} + \text{CH}_3 \leftrightarrow \text{H} + \text{C}_2\text{H}_3$ $\text{CH} + \text{CH}_2\text{O} \leftrightarrow \text{H} + \text{CH}_2\text{CO}$ $\text{H} + \text{CH} \leftrightarrow \text{C} + \text{H}_2$ $\text{CH} + \text{CO}(+\text{M}) \leftrightarrow \text{HCCO}(+\text{M})$ $\text{CH} + \text{CH}_4 \leftrightarrow \text{H} + \text{C}_2\text{H}_4$ $\text{OH} + \text{CH} \leftrightarrow \text{H} + \text{HCO}$ $\text{O} + \text{C}_2\text{H} \leftrightarrow \text{CH} + \text{CO}$ $\text{O} + \text{CH} \leftrightarrow \text{H} 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<p>Absolute Rate of Production B</p> <p> $\text{CH} + \text{O} \leftrightarrow \text{CHO} + \text{B}$ $\text{H}_3\text{O} + \text{B} \leftrightarrow 2\text{H} + \text{OH}$ $\text{H}_3\text{O} + \text{B} \leftrightarrow \text{H}_2\text{O} + \text{H}$ $\text{CHO} + \text{B} \leftrightarrow \text{CO} + \text{H}$ $2\text{O} \leftrightarrow \text{O}_2 + \text{B}$ $\text{O}_2 + \text{B} \leftrightarrow \text{O}_2 + 2\text{B}$ $\text{O} + \text{N} \leftrightarrow \text{NO} + \text{B}$ $\text{NO} + \text{O}_2 \leftrightarrow \text{NO} + \text{O}_2 + \text{B}$ $\text{O} + \text{B} \leftrightarrow \text{O} + 2\text{B}$ $\text{NO} + \text{B} \leftrightarrow \text{NO} + 2\text{B}$ $\text{N} + \text{B} \leftrightarrow \text{N} + 2\text{B}$ $2\text{N} \leftrightarrow \text{N}_2 + \text{B}$ $\text{N}_2 + \text{O}_2 \leftrightarrow \text{NO} + \text{NO} + \text{B}$ $\text{N}_2 + \text{B} \leftrightarrow \text{N}_2 + 2\text{B}$ $\text{NO} + \text{N}_2 \leftrightarrow \text{NO} + \text{N}_2 + \text{B}$ </p> <p> $-1.42\text{E}-15$ $1.39\text{E}-8$ </p>	<p>Absolute Rate of Production B</p> <p> $\text{CH} + \text{O} \leftrightarrow \text{CHO} + \text{B}$ $\text{H}_3\text{O} + \text{B} \leftrightarrow 2\text{H} + \text{OH}$ $\text{H}_3\text{O} + \text{B} \leftrightarrow \text{H}_2\text{O} + \text{H}$ $\text{CHO} + \text{B} \leftrightarrow \text{CO} + \text{H}$ $2\text{O} \leftrightarrow \text{O}_2 + \text{B}$ $\text{O}_2 + \text{B} \leftrightarrow \text{O}_2 + 2\text{B}$ $\text{O} + \text{N} \leftrightarrow \text{NO} + \text{B}$ $\text{NO} + \text{O}_2 \leftrightarrow \text{NO} + \text{O}_2 + \text{B}$ $\text{O} + \text{B} \leftrightarrow \text{O} + 2\text{B}$ $\text{NO} + \text{B} \leftrightarrow \text{NO} + 2\text{B}$ $\text{N} + \text{B} \leftrightarrow \text{N} + 2\text{B}$ $2\text{N} \leftrightarrow \text{N}_2 + \text{B}$ $\text{N}_2 + \text{O}_2 \leftrightarrow \text{NO} + \text{NO} + \text{B}$ $\text{N}_2 + \text{B} \leftrightarrow \text{N}_2 + 2\text{B}$ $\text{NO} + \text{N}_2 \leftrightarrow \text{NO} + \text{N}_2 + \text{B}$ </p> <p> $-1.41\text{E}-15$ $1.19\text{E}-8$ </p>	<p>Absolute Rate of Production B</p> <p> $\text{CH} + \text{O} \leftrightarrow \text{CHO} + \text{B}$ $\text{H}_3\text{O} + \text{B} \leftrightarrow 2\text{H} + \text{OH}$ $\text{H}_3\text{O} + \text{B} \leftrightarrow \text{H}_2\text{O} + \text{H}$ $\text{CHO} + \text{B} \leftrightarrow \text{CO} + \text{H}$ $2\text{O} \leftrightarrow \text{O}_2 + \text{B}$ $\text{O}_2 + \text{B} \leftrightarrow \text{O}_2 + 2\text{B}$ $\text{O} + \text{N} \leftrightarrow \text{NO} + \text{B}$ $\text{NO} + \text{O}_2 \leftrightarrow \text{NO} + \text{O}_2 + \text{B}$ $\text{O} + \text{B} \leftrightarrow \text{O} + 2\text{B}$ $\text{NO} + \text{B} \leftrightarrow \text{NO} + 2\text{B}$ $\text{N} + \text{B} \leftrightarrow \text{N} + 2\text{B}$ $2\text{N} \leftrightarrow \text{N}_2 + \text{B}$ $\text{N}_2 + \text{O}_2 \leftrightarrow \text{NO} + \text{NO} + \text{B}$ $\text{N}_2 + \text{B} \leftrightarrow \text{N}_2 + 2\text{B}$ $\text{NO} + \text{N}_2 \leftrightarrow \text{NO} + \text{N}_2 + \text{B}$ </p> <p> $-3.16\text{E}-16$ $7.04\text{E}-9$ </p>
OF = 45%	OF = 55%	OF = 65%

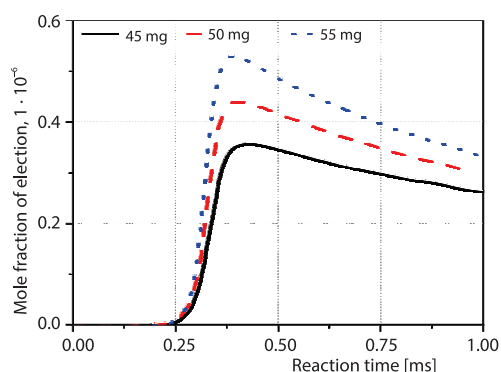


Figure 7. Effect of fuel quantity on in-cylinder electron generation

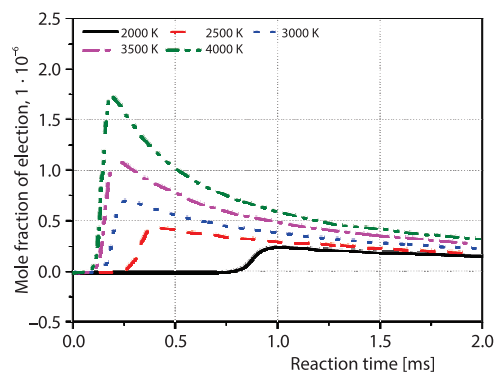


Figure 8. Effect of initial temperature on in-cylinder electron generation

elevated initial temperature. As reported in [32], the ignition delay of hydrocarbon fuel will be shortened as initial temperature increase, in shortened ignition delay lead to advanced maximum in-cylinder electron formation timing. On the other hand, the elevated initial temperature significantly enhanced the reaction rate of propane oxidation as the main oxidation reaction of propane is endothermic [33], the enhancement in propane oxidation leads to increased ionic reaction rates, therefore, lead to an increment in maximum in-cylinder electron mole fraction. The purpose of this investigation under different initial temperature lies in the difference between ICRC and traditional petrol engine operation principle, as a large portion of oxygen is introduced within ICRC engine, the in-cylinder combustion temperature is significantly enhanced, it is also observed by the authors during experiments, the amplitude of detected ion current signal is much larger compare to traditional air intake operation mode [26].

Effect of residual water quantity on in-cylinder electron generation within ICRC engine conditions

The DWI process within ICRC engine can potentially affect in-cylinder electron formation in two ways, DWI within current cycle and t residual water vapor within next cycle. As the experimental results reported in [28], the detected ion current signal amplitude within the first water cycle remains identical compare to dry cycle, and the detected ion current signal amplitude within the 2~5 cycles after DWI deactivation still presents similar characteristics

to enhanced in-cylinder combustion, however, the formation of CH is decreased, therefore, lead to a slightly decrement in in-cylinder mole fraction of electron which indicate that the amplitude of detected ion current signal amplitude will diminish.

The effect of fuel quantity on in-cylinder electron generation is illustrated in fig. 7. As it can be seen in the figure, the mole fraction of in-cylinder electron increased significantly as fuel quantity increased, this result indicates that the detected ion current signal amplitude within ICRC engine under elevated engine load will be enhanced, which is consistent with the experimental results reported in [26]. Analysis suggest that the enhancement of in-cylinder electron generation is caused by the increment of in-cylinder propane content, as the mole fraction of propane increased, the formation of CH radical is improved, therefore, as the most important primary reactant of electron generation, the in-cylinder electron formation is enhanced.

Meanwhile, the effect of initial temperature on in-cylinder electron generation is also investigated. As presented in fig. 8, the initial temperature shows great impact on in-cylinder electron formation, the maximum electron mole fraction and its timing are both enhanced under

compare to water cycle, these phenomenon implies that the variation of detected ion current signal is mainly driven by residual water vapor. Therefore, the initial composition is altered into combination of propane, O_2 , CO_2 , and water vapor to simulate the in-cylinder composition during ICRC engine operation.

Figure 9 illustrates the effect of residual water quantity on in-cylinder propane consumption. As it can be seen in the figure, the increment in initial residual water vapor content show positive effect in propane oxidation, the consumption rate of propane is enhanced as residual water quantity increased. This phenomenon is contradictory to the common sense that in-cylinder water vapor normally acts as an obstruction for better hydrocarbon oxidation. To better explain this phenomenon, the main reactions of H_2O and their absolute rate of production under different timing of propane consumption is calculated, the detailed results are presented in tab. 4. It is worth noting that the OH is a key reaction radical as propane gets oxidized, at 1% propane consumption, the introduction of water vapor is capable of providing massive OH radical as the reverse production rate of reaction $OH + HO_2 \rightleftharpoons O_2 + H_2O$ is dominant. When the oxidation of propane carried out, at 5% propane consumption, the water vapor reacts with intermediate radicals including HO_2 , O_2 , CH_3 , H , *etc.* which further provides additional OH radical to facilitate the propane oxidation reaction $OH + C_3H_8 \rightleftharpoons C_3H_7 + H_2O$, therefore, the introduction of DWI process helps to improve propane oxidation which results in a quicker propane consumption rate compare to dry cycle.

Meanwhile, the effect of temperature on in-cylinder electron generation is not included in the previous calculation while DWI shows significant impact. According to [23, 26], the in-cylinder temperature decreased as DWI involves. The negative effect of DWI on in-cylinder temperature can be concluded as two aspects, physically and chemically. On the physical aspect, the injected water absorbs combustion heat because of its latent heat, on the other hand, the generated steam deteriorated in-cylinder specific heat capacity, which is also discussed and proved in [34]. As for the chemical aspect, the calculation results of propane mole fraction variation trends under different initial temperature with or without DWI is presented in fig. 10. As it can be seen in the figure, the residual water vapor significantly decreased propane oxidation under 2000 K initial temperature compare to 2500 K initial temperature. This result can be utilized to explain two phenomenon, the first one is enhancement of ion current signal during ICRC engine experiments as reported in [26], which is caused by the propane oxidation improvement results in large content of CH radical formation. The second one is as observed during experiments, the ion current signal decreased rapidly as DWI quantity increased, this is mainly caused by the

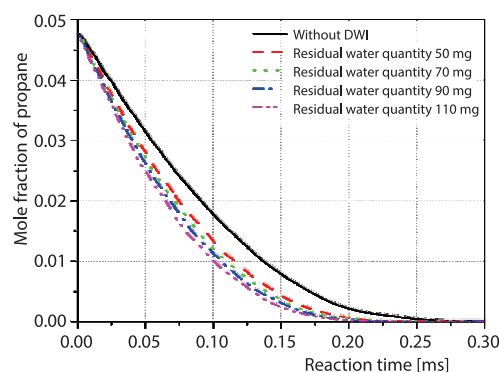


Figure 9. Effect of residual water quantity on in-cylinder propane consumption

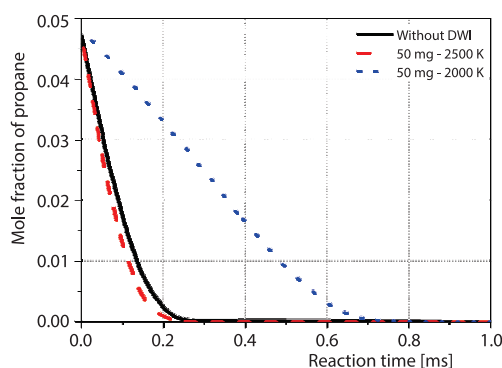


Figure 10. Effect of in-cylinder temperature on in-cylinder propane consumption under DWI

Table 4. Comparison of H₂O reactions and reaction rate between DWI and without DWI within ICRC engine condition

Propane consumption	Without DWI	With DWI
1%	<p>Absolute Rate of Production H₂O</p> <p>OH+C₃H₈⇌C₃H₇+H₂O CH₂(S)+O₂⇌CO+H₂O OH+CH₃⇌CH₂(S)+H₂O OH+CH₃⇌CH₂+H₂O OH+HO₂⇌O₂+H₂O H+HO₂⇌O+H₂O</p> <p>2.92E-10 6.25E-4</p>	<p>Absolute Rate of Production H₂O</p> <p>OH+HO₂⇌O₂+H₂O OH+CH₄⇌CH₃+H₂O OH+H₂O₂⇌HO₂+H₂O OH+C₃H₈⇌C₃H₇+H₂O OH+C₂H₆⇌C₂H₅+H₂O OH+H₂⇌H+H₂O</p> <p>6.13E-2 3.84E-3</p>
5%	<p>Absolute Rate of Production H₂O</p> <p>OH+C₃H₈⇌C₃H₇+H₂O OH+CH₃⇌CH₂(S)+H₂O CH₂(S)+O₂⇌CO+H₂O OH+CH₃⇌CH₂+H₂O OH+HO₂⇌O₂+H₂O OH+C₂H₄⇌C₂H₃+H₂O</p> <p>3.18E-1 5.18E-2</p>	<p>Absolute Rate of Production H₂O</p> <p>OH+C₃H₈⇌C₃H₇+H₂O OH+H₂O₂⇌HO₂+H₂O OH+HO₂⇌O₂+H₂O OH+CH₄⇌CH₃+H₂O OH+H₂⇌H+H₂O OH+C₂H₆⇌C₂H₅+H₂O</p> <p>6.12E-2 6.38E-2</p>
10%	<p>Absolute Rate of Production H₂O</p> <p>OH+C₃H₈⇌C₃H₇+H₂O OH+CH₃⇌CH₂(S)+H₂O OH+HO₂⇌O₂+H₂O CH₂(S)+O₂⇌CO+H₂O OH+CH₃⇌CH₂+H₂O OH+C₂H₄⇌C₂H₃+H₂O</p> <p>3.64E-1 1.22E-1</p>	<p>Absolute Rate of Production H₂O</p> <p>OH+C₃H₈⇌C₃H₇+H₂O OH+H₂O₂⇌HO₂+H₂O OH+H₂⇌H+H₂O OH+CH₄⇌CH₃+H₂O OH+HO₂⇌O₂+H₂O OH+C₂H₆⇌C₂H₅+H₂O</p> <p>1.59E-1 2.91E-1</p>
50%	<p>Absolute Rate of Production H₂O</p> <p>OH+C₃H₈⇌C₃H₇+H₂O OH+HO₂⇌O₂+H₂O OH+CH₃⇌CH₂(S)+H₂O OH+C₂H₄⇌C₂H₃+H₂O OH+CH₂O⇌HCO+H₂O OH+CH₃⇌CH₂+H₂O</p> <p>2.41E-5 1.35E0</p>	<p>Absolute Rate of Production H₂O</p> <p>OH+C₃H₈⇌C₃H₇+H₂O OH+CH₃⇌CH₂(S)+H₂O OH+H₂O₂⇌HO₂+H₂O OH+HO₂⇌O₂+H₂O OH+C₂H₄⇌C₂H₃+H₂O OH+CH₄⇌CH₃+H₂O</p> <p>2.74E-1 1.74E0</p>
100%	<p>Absolute Rate of Production H₂O</p> <p>OH+H₂⇌H+H₂O 2OH⇌O+H₂O OH+CH₂O⇌HCO+H₂O OH+HO₂⇌O₂+H₂O OH+CH₂⇌CH+H₂O OH+HCO⇌H₂O+CO</p> <p>1.9E-1 6.99E0</p>	<p>Absolute Rate of Production H₂O</p> <p>OH+H₂⇌H+H₂O OH+CH₂O⇌HCO+H₂O 2OH⇌O+H₂O OH+HO₂⇌O₂+H₂O OH+CH₂⇌CH+H₂O OH+HCO⇌H₂O+CO</p> <p>2.37E-1 8.68E0</p>

negative effect of in-cylinder temperature during water evaporation, as the amount of injection water increased, the in-cylinder temperature is significantly decreased, therefore, lead to a rapid reduction in detected ion current signal.

Furthermore, the effect of residual water quantity on in-cylinder electron generation under 2500 K initial temperature is calculated and presented in fig. 11. To be noted that, the negative effect of DWI on in-cylinder temperature is not considered as this section mainly focused on the chemical effect of residual water vapor on in-cylinder electron formation. As it can be seen in the figure, the generated electron increased as residual water quantity elevated, meanwhile, the timing of peak electron generation is also advanced. This numerical result is capable in explaining the enhanced detected ion current signal during ICRC engine experiments.

Analysis suggest that, the introduction of water vapor (without consideration of in-cylinder temperature decrement) is beneficial in providing extra OH radical which facilitates in propane oxidation, as the reaction rate of propane oxidation enhanced, the formation of CH is improved, therefore, lead to larger and earlier in-cylinder electron generation.

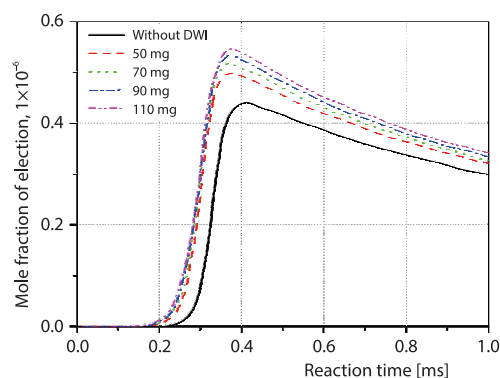


Figure 11. Effect of DWI on in-cylinder electron generation

Outlook

The reported work mainly focused on utilizing 0-D chemical kinetic analysis to reveal the fundamental chemical mechanism of unprecedented ion current signal variation within ICRC engine reported in [26]. The complex interactions between oxy-fuel combustion and DWI process is ignored as the 0-D calculation can hardly involve multiple water droplets evaporation, on the other hand, the negative impact of DWI on in-cylinder temperature is simplified into a uniform effect, while in reality the in-cylinder water distribution is highly heterogeneous and its effect on temperature drop varies significantly. Therefore, further verification and calculation under 3-D simulation considering both fluid dynamic and chemical kinetics is needed, by doing so, the actual variation of in-cylinder electron formation under ICRC engine condition with DWI can be revealed. This simulation work is currently ongoing which is expected to obtain some key mechanism and phenomenon in near future.

Conclusions

In this paper, a brief literature review of ICRC was first conducted to demonstrate the feasibility of ultra-high efficiency and zero emission powertrain, while the in-cylinder feedback signal is needed for better close-loop control of in-cylinder oxy-fuel combustion, as ion current detection is utilized to fulfill this requirement, an unprecedented variation in ion current signals were observed, to better understand this phenomenon and provide fundamental information for chemical interactions between in-cylinder water vapor and electron generation, a 0-D chemical kinetic model is established within Chemkin-Pro, the effect of intake OF, fuel quantity, initial temperature and in-cylinder water vapor on propane oxidation and electron formation were conducted, the conclusions of this work are presented as follows.

- The intake OF show significantly impacts on in-cylinder temperature, the elevated in-cylinder temperature is observed at increased intake OF, this enhancement in in-cylinder temperature is related to elevated oxygen content which lead to faster propane oxidation and optimized in-cylinder heat capacity.

- The most important species regarding to electron formation is CH, the elevated intake OF lead to larger portion of CH formation therefore, lead to increment in rate of production of electron. This calculation results are in consistent with ICRC engine experiment.
- The fuel quantity and initial temperature both show positive effect in in-cylinder electron formation, as the rate of production of electron is enhanced under elevate CH formation.
- Contradictory to the common reported negative impact of in-cylinder water vapor on fuel oxidation, the residual water vapor shows positive effect in providing additional OH radical which facilitate in propane oxidation. The most important reactions related to OH formation includes $\text{OH} + \text{HO}_2 \rightleftharpoons \text{O}_2 + \text{H}_2\text{O}$ and other reactions between H_2O and HO_2 , O_2 , CH_3 , and H as described in this paper.
- The initial temperature is a vital parameter which determines the residual water vapor show positive or negative effect on propane oxidation, this conclusion can be utilized to explain enhancement of ion current signal during ICRC engine experiments and rapid ion current signal decrement as DWI quantity increased.
- The formation of electron is enhanced under residual water vapor involvement, the maximum electron formation and its timing are both enhanced, which is in consistent with the experimental results reported in previous study. To be noted that, this conclusion can only be drew under certain in-cylinder temperature, the in-cylinder electron under DWI may decrease as in-cylinder temperature drops.
- Further 3-D simulation combining fluid dynamic and chemical kinetics is needed to lucubrate the complex interactions between oxy-fuel combustion and DWI process, which further determines the actual in-cylinder electron formation.

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Nomenclature

Acronyms

BTE – brake thermal efficiency
 CI – compression ignition
 DWI – direct water injection
 EGR – exhaust gas re-circulation
 fTDC – firing top dead center
 FCV – fuel cell vehicle

HCCI – homogeneous charge compression ignition
 ICE – internal combustion engine
 ICRC – internal combustion Rankine cycle
 OF – oxygen fraction
 SI – spark ignition
 TTW – tank-to-wheel

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