



INTERNATIONAL JOURNAL OF CREATIVE RESEARCH THOUGHTS (IJCRT)

An International Open Access, Peer-reviewed, Refereed Journal

Synergistic Effects Of Zinc Nanoparticles On RCCI Engine Performance- CFD Analysis

SK. Avinash Kapil^{1*}, Peketi Sri Satya Sai Anil², Madabathula Gandhi Venkata Simha Dhanush³, Bugatha Sunil⁴, Brehara Vamsikrishna⁵

^{1*} Assistant professor, Mechanical Engineering Department, Godavari Institute of Engineering & Technology(A), Rajamahendravaram, India.

² Graduate student, Mechanical Engineering Department, Godavari Institute of Engineering & Technology(A), Rajamahendravaram, India.

³ Graduate student, Mechanical Engineering Department, Godavari Institute of Engineering & Technology(A), Rajamahendravaram, India.

⁴ Graduate student, Mechanical Engineering Department, Godavari Institute of Engineering & Technology(A), Rajamahendravaram, India.

⁵ Graduate student, Mechanical Engineering Department, Godavari Institute of Engineering & Technology(A), Rajamahendravaram, India.

Abstract

This analysis study explores the effects of Zinc nanoparticles as additives in a Reactivity Controlled Compression Ignition (RCCI) engine fueled with methane (CH₄) and diesel. The research focuses on combustion characteristics, performance improvements, and emission variations. Simulations were conducted using CONVERGE CFD, with RNG k-ε turbulence model and SAGE Detailed Chemistry. Performance analysis of Diesel with 100PPM of Zn nanoparticles M/DI50/Zn100 were compared with pure diesel DI100, premixed methane 50% and diesel M/DI50 shows significant increase of Indicated power by 4%, thermal efficiency by 5%, BSFC reduced by 3% and emissions contents CO, CO₂, NO_x reduced by 32%, 15%, 16% respectively but HC is increased by 231%. Overall results indicate that Zn enhances combustion efficiency significantly and increase peak pressure along with high HRR. In addition Zn reduces greenhouse gases like CO, CO₂ significantly.

Keywords: Zn nanoparticles, RCCI, Converge CFD, RNG k-ε, SAGE, Combustion, Emissions

1. Introduction

In view of raising environmental crisis, counter measures to reduce emissions from transport industry is indispensable necessity along with economic benefit. Reactivity Controlled Compression Ignition (RCCI) is capable of achieving fuel efficiency and near zero emission simultaneously. RCCI uses LRF (low reactive fuel) like gasoline, methanol, CNG and HRF (high reactive fuel) through which the combustion will be carried out in low temperature and maintain efficiency.

Physical and chemical properties of Zn nanoparticles promises best outcomes in terms of combustion efficiency and counter measures for emissions. Studies shows that nanoparticles can act as catalyst and combustibles. Heat capacity (c_p) 25.39 J/mol K and thermal conductivity 116 W/m K increases fuel-air mixture which promotes better heat transfer rate inside combustion chamber and also reduces ignition delay. Since Zn nanoparticles have high surface area with 20nm size, surface catalytic effect breakdowns hydrocarbons into reactive radicals (OH, HO₂, H, CH₃), further Zn enhances conversion of CH₄ > CH₃ > CO > CO₂.

This study focuses on modelling enriched Methane and Diesel blend with high cetane number due to addition of Zn Nano additives, the base line simulation and reaction mechanisms data is taken from Rahimi, A et. Al [8], the 60° sector geometry model is solved in Converge CFD with AMR and complete SAGA chemistry solver. In order to account for methane gas the quantity of diesel is considered half of total quantity injected for pure diesel case. RNG k- ϵ turbulence model and SAGE Detailed Chemistry is employed in Converge Studio with 78 species, 468 reactions. Results are compared with baseline simulation in terms of engine performance and emissions.

2. Literature review

Kokjohn, Sage, et al.[1] [2] proposed RCCI engine which used blends of low reactive fuels (gasoline, natural gas, and alcohol fuel) which are premixed with air or EGR gases through intake port injection and high reactive fuels (diesel, biodiesel) for pilot injection late in the compression stroke. This concept of dual fuel shown better control on combustion rather than other strategies like HCCI and PCCI. Various researches carried out by Reitz, Rolf D.,[3] studied RCCI engine for clean reactivity, Hosseini, Seyyed Hassan, et al. [4] worked on hydrogen in dual fuel engine, Xu, Leilei, et al [5] worked with ammonia in marine diesel fuel, Krishnamoorthi, M., et al. [6] reviewed on low combustion engine, Li, J., et al. [7] experimented RCCI with fuel ratios and injection timing.

Rahimi, A et. Al [8] studied dual fuel engines using n-heptane and methane for better control on combustion. As a result an optimized kinetic mechanism for dual fuel consisting of n-heptane and methane is developed, which includes 76 species and 464 reactions. These reaction mechanism doesn't count any activity less than 600K in order to reduce computation time. Further stated that increase of natural gas concentration in the combustion volume is less effective compared to diesel combustion.

M Nazemi, M Shahbakhti [9] 3D-CFD of RCCI engine using converge is developed and validated against experimental data. CFD model is analysed through CA10, CA50, CA90 is effective in accounting RCCI combustion since they are hard for comparison. Results show that injection spray angle $>55^\circ$ and PR 0.76 yielded best combustion parameters. Augmenting the fuel impingement force via elevated compression ratios and injection pressures, coupled with a temporal advancement of the start of injection, has been observed to yield ameliorative effects upon the production of unburnt hydrocarbon and carbon monoxide effluents. CFD model is analysed through CA10, CA50, CA90 is effective in accounting RCCI combustion since they are hard for comparison.

Zhou, Dezhi, et al [10] analyzed CTC-CHEMKIN model in RCCI mode. The application of this model reduced computational time by 20% than sole CHEMKIN solver. Hamdi et al [11] conducted simulations to enhance engine efficiency and reduce pollutant emissions by analysing the impact of the equivalence ratio (ϕ) on natural gas (NG)/heptane-fuelled combustion using a validated numerical model in ANSYS Forte under the RANS framework and demonstrates that $\phi = 0.6$ offers a balance between fuel efficiency and lower emissions while validating the numerical model against experimental data. Poorghasemi, Kamran, et al. [12] studied effects of different parameters PR, SOI and spray angles. NG/Diesel is simulated in Converge CFD model and results showed increasing PR reduces combustion rate due to lower reactivity of Methane and narrow spray angle have elevated values of HC and CO emissions.

Ebrahiem Esmail, et al. [13] studied improvements in diesel engine by adding Zinc oxide nanoparticles as fuel additive. Based on experiments concluded ZnO increases cetane number resulting remarkable combustion efficiency and reduction in BSFC. CO emissions are reduced upto 40PPM and has no effect during further addition. Indeed CO₂ and NO_x levels are increased. HC emissions are in near zero fraction.

De Robbio, Roberta, and Ezio Mancaruso [14] analyzed dual fuel combustion enriched with hydrogen at low speed with CFD and validated through optical methods. Simulations are performed with the ANSYS Forte® code. Turbulence is simulated via the RANS RNG k- ϵ , the atomization of the liquid jet and following break-up are modelled via the Kelvin-Helmholtz/Rayleigh-Taylor (KH-RT) hybrid model. The quantitatively comparison between the main pollutant emissions, i.e. CO, CO₂, UHC and NO_x, confirms the reliability of numerical kinetic model at a reduced load and the effective reduction of this pollutant emissions. The results from their work reflect high reliability on numerical methods to predict and analyze emissions which will enhance the scope of research and better solution through CFD.

3. Methodology

3.1 Computational model

The combustion engine model replicates Caterpillar SCOTE [Table 1]. Since the complete 360° engine uses 6 nozzle symmetrically placed around the injector, therefore 60° sector is generated using engine sector tool within the converge studio for effectively reduce the computation time and obtain precise results. The surface geometry generated is section of engine cylinder which includes the head, wall, piston, and two periodic face boundaries represent the plane of cut. Crank angle based IC engine parameter is considered

along with transient solver for run parameters. Fuels are often simulated using surrogate method to reduce reaction time and complexity of computation of model, in this case CH₄ and n-heptane represents natural gas and diesel as surrogates, whereas Zn is introduced in dispersion method to mix with combustion contents effectively. Simulation uses cyclic 720° configuration of total crank rotation i.e., from -360° to 360°. Fig 1 (Top view) & Fig 2 (Front view) from generated sector.

TABLE 1 Engine details used for modelling

Base engine type	Caterpillar SCOTE
Bore X stroke	13.72 X 16.51 cm
Connecting rod length	26.16cm
Squish height	0.157cm
Piston pin offset	None
Displacement	2.44 L
Geometric comp. ratio	16.1:1
Swirl ratio	0.7
Bowl type	Open crater
Number of valves	4
IVO	-335ATDC
IVC	-85 and -143 ATDC
EVO	130ATDC
EVC	-355ATDC

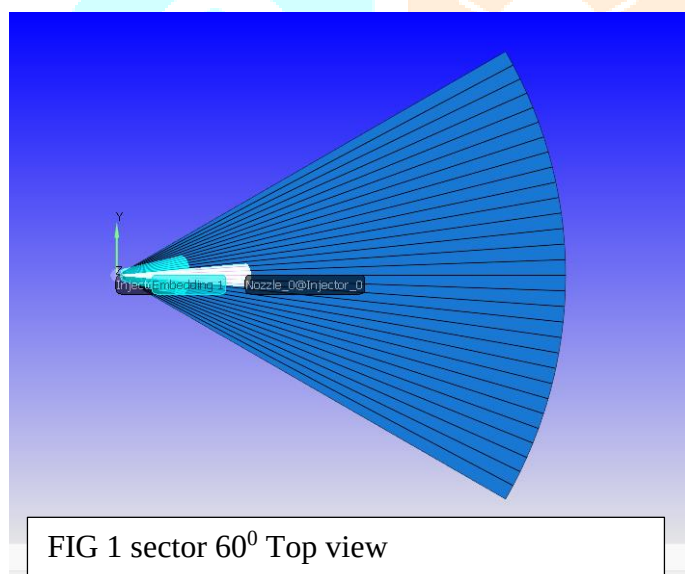


FIG 1 sector 60° Top view

3.2 Injection strategy

Computation is carried out in three different case setups namely DI100, M/DI50, M/DI50/Zn100, table 2 represents case matrix used for this study, since the computation time is considerable large this study only explores Zn effects at 100 PPM.

Table 2 Case setup matrix for simulations

Test Case	Fuel Composition	Injection Strategy	Parameters to Measure
DI100	Diesel	RCCI (pilot)	Combustion phasing (CA50), pressure, HRR
M/DI50	50% Methane, Diesel	RCCI (port + pilot)	CO, NO _x , HC, soot, efficiency
M/DI50/Zn100	50% Methane, Diesel + 100 PPM Zn	RCCI (port + pilot)	Baseline emissions and combustion data

3.3 Combustion and reaction mechanism

Combustion model employs SAGE detailed chemistry solver which is proven to solve complex chemical kinetics, KH-RT breakup model is utilized for spray atomization for diesel injection. For effective implication of turbulence RNG k-ε model is used for mixing of fuels accurately, turbulent Prandtl number set to 0.9 and Schmidt number 0.79 with maximum turbulent viscosity allowed in the combustion domain 10 N.s/ m². Combustion solver is enabled after -10° such that computational time is reduced and cut off temperature is set to 600K.

Species Zn & ZnO is defined in solid species with their thermal properties as per NASA 7-Coefficient polynomial, for the given temperature range T:

$$\frac{C_p}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$\frac{H}{RT} = a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T}$$

$$\frac{S}{R} = a_1 \ln(T) + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7$$

Where, C_p = Specific heat at constant pressure, H = Enthalpy, S = Entropy, R = Universal gas constant (8.314 J/mol·K), a₁ to a₇ = Polynomial coefficients, T = Temperature (K)

Reaction mechanism uses Arrhenius expression, the rate of chemical reaction is given as:

$$k = AT^b e^{(-\frac{E_a}{RT})}$$

Where, k = Rate constant (mol, cm³, s units depend on reaction order), A = Pre-exponential factor (frequency of collisions), b = Temperature exponent, E_a = Activation energy (J/mol or cal/mol)

3.4 AMR and Mesh strategy

Basic grid size of 1.4mm for entire computational domain which is 158048 base cell count. Converge adopts Adaptive Mesh Refinement (AMR) with temperature gradient to capture HR zones accurately and velocity gradient for flame jet dynamics, Sub grid Scaling is used for effective tracking the model

3.5 Boundary and Initial conditions

Cylinder simulation starts from -147° i.e. start of compression stroke after BDC. Premixed charge with mass fraction of 0.02282932. The initial conditions of combustion chamber is as follows temperature 355K, pressure 134793 bar along with turbulent kinetic energy $62.0271 \text{ m}^2/\text{s}^2$ and turbulent dissipation $17183.4 \text{ m}^2/\text{s}^2$. Diesel is injected with single injector with SOI as -9° and duration of injection is 10.5° and total injected mass of $1.35083\text{e-}05 \text{ kg}$ in case M/DI50, M/DI50/Zn100.

3.6 Simulation parameters

Sector RNS simulation is carried at an engine speed of 1600 RPM. Run parameters obey transient, crank angle-based engine simulation, with simulation mode as fully hydrodynamic and gas flow solver as compressible, liquid flow solver as incompressible. Time step calculation follows variable time-step algorithm with initial time step $5\text{e-}07\text{s}$, minimum and maximum time step as $1\text{e-}08$, $2.5\text{e-}05$ respectively.

4. Validation and Results

Simulations are carried out on same physical parameters, initial and boundary conditions. Variable parameters for solution is species, parcels and mass fraction. IMEP is calculated with expression

$$\text{IMEP} = \frac{\text{Gross work}}{\text{Displacement volume}}$$

Since displacement volume is constant with $V = 2.44\text{E-}03$. Table 3 and Fig3 show constant value of volume through all 3 simulations.

Table 3 Details of Gross work, IMEP, Displaced volume

Description test case	Gross Work (N*m)	IMEP (gross) (Pa)	Displaced volume (m^3)
DI100	3396	$1.39\text{E+}06$	$2.44\text{E-}03$
M/DI50	3307	$1.35\text{E+}06$	$2.45\text{E-}03$
M/DI50/Zn100	3328.5	$1.36\text{E+}06$	$2.44\text{E-}03$

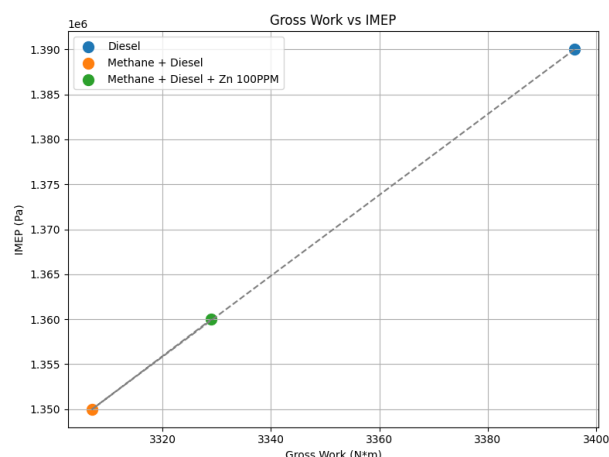


Fig 3 Gross work vs IMEP for 3 cases

Engine performance is compared in terms of gross work, IMEP, CAD10, CAD50, CAD90, PFP, HRR. Methane surrogate with 50% mass compensation that of diesel reduces the key performances compared to pure diesel case but with addition of Zn Nanoparticles, values are boosted and overcome drawbacks of methane and diesel case. The detailed comparison is shown in Table 4.

Table 4 Comparison of engine performance results

Description of fuel	CAD from	CAD to	TDC firing	Gross Work	IMEP (gross)	CAD 10				HRR Peak
	(deg)	(deg)	(deg)	(N*m)	(Pa)	(deg)	(deg)	(deg)	(Mpa)	(J/deg)
DI100	- 141.2	- 135	- 0.01	- 3396	- 1.39E+06	- 1.2	- 13.01	- 29.25	- 11.07	- 665.2
M/DI50	- 141.2	- 135	- 0.002	- 3307	- 1.35E+06	- 0.405	- 7.514	- 32.53	- 11.06	- 649.2
M/DI50/Zn100	- 141.2	- 135	- 0.005	- 3328.5	- 1.36E+06	- 0.198	- 6.8	- 31.65	- 11.11	- 681.66

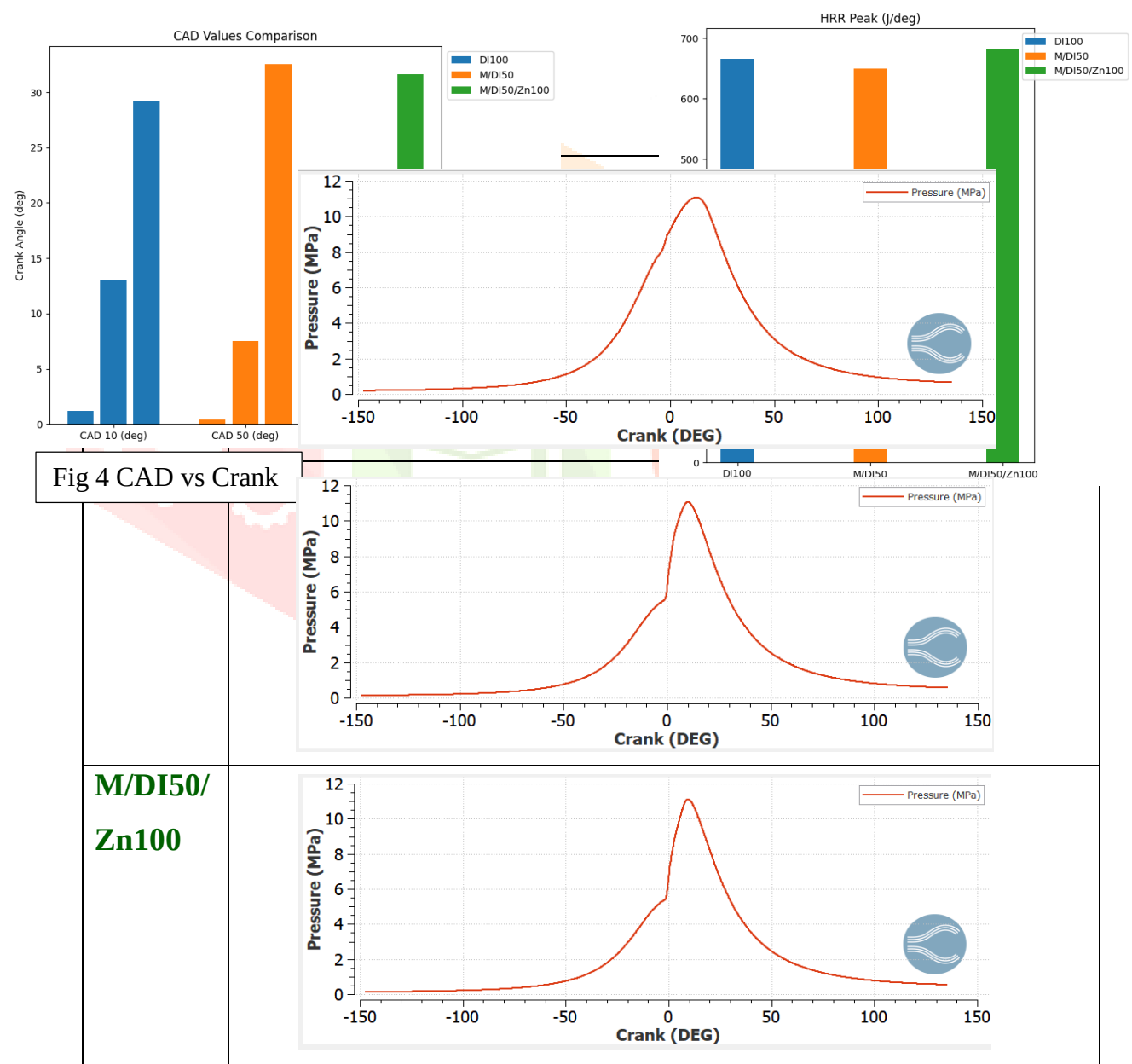


Fig 6 comparison of cylinder pressure vs Crank (deg)

Comparing with the simulation results with three different fuel proportions, the effect of Zn is not went unnoticed, In Fig 4, SOI started early in crank degrees, such that the radicals will have high duration to react

and improve combustion efficiency is improved. Methane being low reactive reduced the HRR and addition of Zn overcame that drawback Fig 5. Pressure variation can also be noticed during SOI just around TDC Fig 6.

Emissions from three cases are visualized in Fig 7 (CO and CO₂ vs crank angle) shows that the amount of both green house gases are reduced. The amount of pollution caused by diesel is significantly reduced by methane composition but with addition of zinc has further reduced the quantities. Oxide radicals are well reacted with our target parcels and provided with better outcomes.

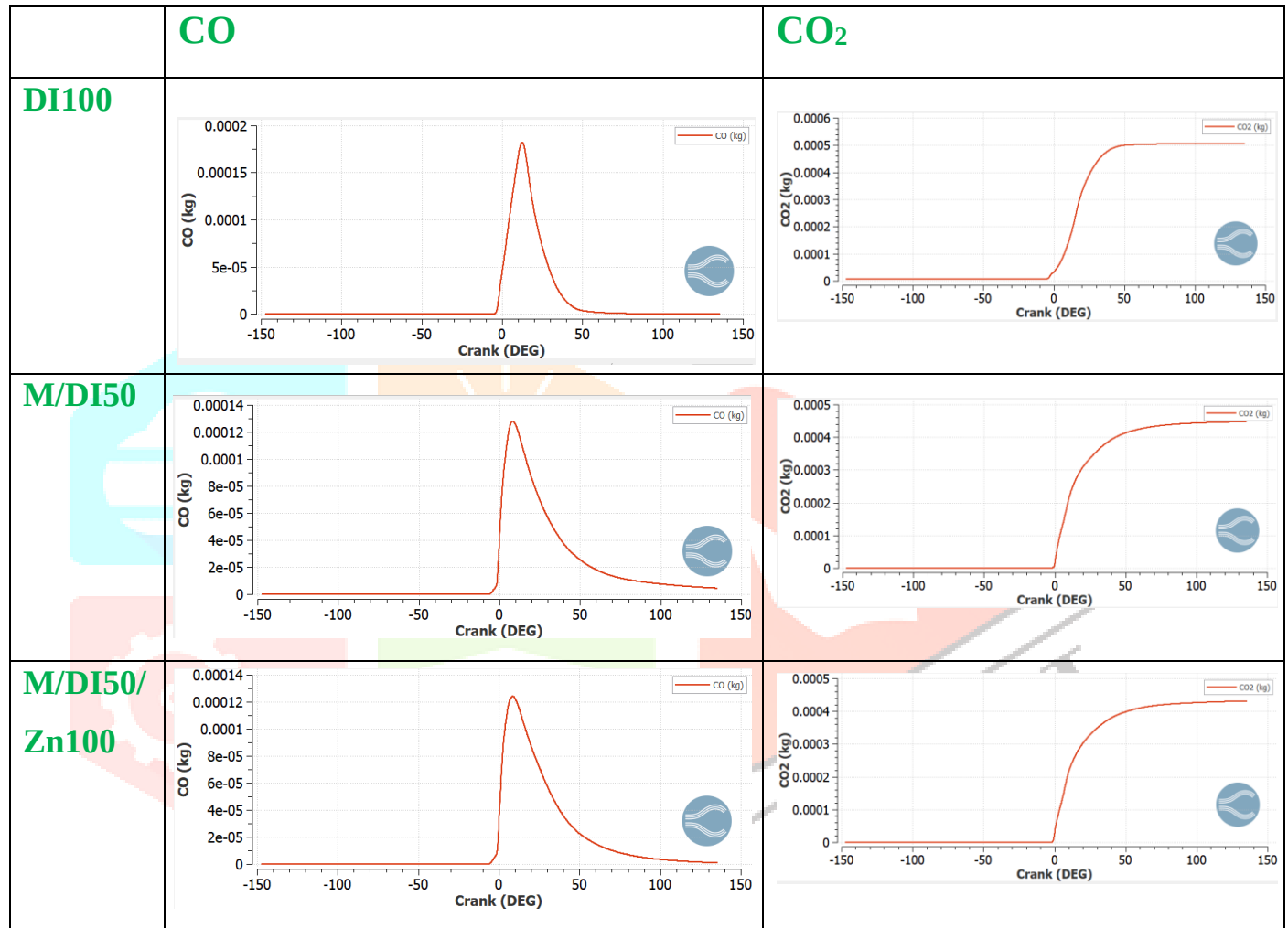
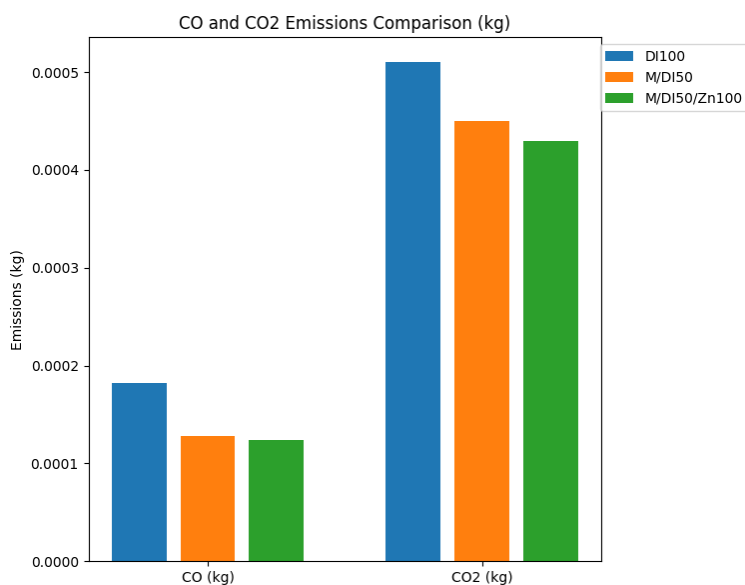
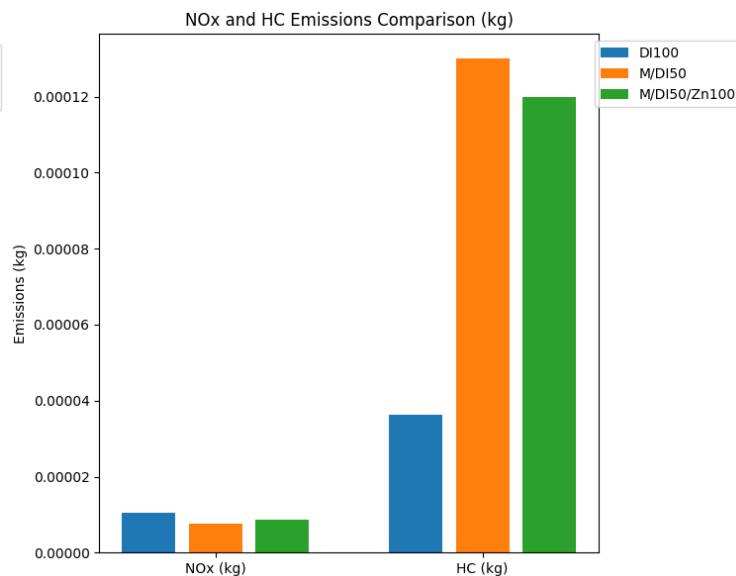


Fig 7 CO, CO₂ emissions vs Crank in different cases

Methane contribution in combustion have added more hydrocarbon contents due to the premixture quantity. Reaction radicals OH, H are significantly abundant in reaction, which has led to formation of higher HC content in emissions. HC content is noticeable increased in M/DI50 but with addition of Zn i.e. M/DI50/Zn100 case it reduced to 25% when compare with DI100 its quantity is extreme. NO_x quantity has lowest value in M/DI50 case and slightly increase with Zn but lower than DI100.

Table 5 Comparison of Emission exhausted from engine model in different cases.

Emission	DI100 (kg)	M/DI50 (kg)	M/DI50/Zn100 (kg)	Change: M/DI50 vs DI100	Change: M/DI50/Zn100 vs DI100
NOx	1.05E-05	7.67E-06	8.78E-06	↓ 26.95%	↓ 16.38%
HC	3.62E-05	0.00013	0.00012	↑ 259.39%	↑ 231.49%
CO	0.000182119	0.000128033	0.000124058	↓ 29.70%	↓ 31.87%
CO ₂	0.00051	0.00045	0.00043	↓ 11.76%	↓ 15.69%

**Fig 8 CO and CO₂ emissions in different cases****Fig 9 NOx and HC emissions in different cases**

5. Conclusions

Counter measures to reduce diesel combustion emissions, the approach with Natural gas and Zn nanoparticles have shown significant improvement in combustion efficiency and HRR. In conclusion

1. CO emissions are reduced to 31.87% compared to DI100 indicates improved oxidization with zinc, CO₂ reduction of 15.69% suggests enhanced combustion efficiency.
2. NOx control of 16.38% vs DI100 is significant progress with dual fuel mode, HC content is tediously increased up to 230% when compared to single fuel emission.
3. Methane (M/DI50) reduces NOx, CO, and CO₂, but significantly increases HC emissions. Zinc (M/DI50/Zn100) further reduces CO and CO₂, while NOx slightly increases compared to M/DI50, but still remains lower than DI100

Overall dual fuel RCCI engine with NG-Diesel added with Zn nanoparticles improves combustion efficiency and reduce most emissions, except HC.

6. Future scope

- In continuation to the CFD work, Zn and ZnO Nanoparticles to be experimentally analyzed and optimized for consistent PPM quantity.
- Working with different Nano additives along with biodiesel and hydrogen cases.

References

- [1] Kokjohn, Sage, et al. "Fuel reactivity controlled compression ignition (RCCI) combustion in light-and heavy-duty engines." SAE International Journal of Engines 4.1 (2011): 360-374.
- [2] Kokjohn, Sage Lucas. Reactivity controlled compression ignition (RCCI) combustion. Diss. The University of Wisconsin-Madison, 2012.
- [3] Reitz, Rolf D., and Ganesh Duraisamy. "Review of high efficiency and clean reactivity controlled compression ignition (RCCI) combustion in internal combustion engines." Progress in Energy and Combustion Science 46 (2015): 12-71.
- [4] Hosseini, Seyyed Hassan, et al. "Use of hydrogen in dual-fuel diesel engines." Progress in Energy and Combustion Science 98 (2023): 101100.
- [5] Xu, Leilei, et al. "Performance and emission characteristics of an ammonia/diesel dual-fuel marine engine." Renewable and Sustainable Energy Reviews 185 (2023): 113631.
- [6] Krishnamoorthi, M., et al. "A review on low temperature combustion engines: Performance, combustion and emission characteristics." Renewable and Sustainable Energy Reviews 116 (2019): 109404.
- [7] Li, J., et al. "Effects of fuel ratio and injection timing on gasoline/biodiesel fueled RCCI engine: A modeling study." Applied Energy 155 (2015): 59-67.
- [8] Rahimi, A., E. Fatehifar, and R. Khoshbakhti Saray. "Development of an optimized chemical kinetic mechanism for homogeneous charge compression ignition combustion of a fuel blend of n-heptane and natural gas using a genetic algorithm." Proceedings of the institution of mechanical engineers, Part D: Journal of Automobile Engineering 224.9 (2010): 1141-1159.
- [9] Nazemi, M., and M. J. A. E. Shahbakhti. "Modeling and analysis of fuel injection parameters for combustion and performance of an RCCI engine." Applied Energy 165 (2016): 135-150.
- [10] Zhou, Dezhi, et al. "Efficient combustion modelling in RCCI engine with detailed chemistry." Energy Procedia 105 (2017): 1582-1587.
- [11] Hamdi, Fathi, Wassim Harizi, and Mouldi Chrigui. "RANS Study on the Impact of Equivalence Ratio on Natural Gas/Diesel-Fueled Combustion in RCCI Engine." Journal of Applied and Computational Mechanics (2025).

- [12] Poorghasemi, Kamran, et al. "Effect of diesel injection strategies on natural gas/diesel RCCI combustion characteristics in a light duty diesel engine." *Applied energy* 199 (2017): 430-446.
- [13] Ebrahiem, Ebrahiem Esmail, et al. "Improvement of diesel fuel to enhance engine performance and emissions using zinc oxide nanoparticle additive." *Egyptian Journal of Chemistry* 65.2 (2022): 349-355.
- [14] De Robbio, Roberta, and Ezio Mancaruso. "Hydrogen combustion analysis via infrared and visible optical diagnostics combined with CFD in a dual fuel engine at low load." *International Journal of Hydrogen Energy* 81 (2024): 418-435.

