Investigating HCCI Engine Operating Parameters Under the Simultaneous Dual Fueling of Ammonia and Hydrogen Based on Detailed Chemical Kinetics Modelling

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Abstract. Challenges associated with the homogeneous charge combustion ignition (HCCI) concept includes combustion phasing control and a narrow operating window. To address the HCCI engine developmental needs, chemical kinetic solvers have been recently included in the commercial engine simulation toolchains like GT-Suite v2022. Their applicability has not been thoroughly tested, especially when less-conventional fuel options have been considered. The purpose of this study is to test the feasibility of kinetic solvers included in the GT-Suite, for simulating HCCI combustion with multi-component fuel blend, consisting predominantly of ammonia, NH_3, and hydrogen, H_2. The study investigated the effect of fuel blending, air to fuel equivalence ratio, and compression ratio on a dual-fuel 1-cyclinder HCCI engine model. Key combustion parameters such as peak pressure, heat release rate, start of combustion were analyzed. Feasibility of the simulations have been validated by benchmarking the results against the base-line HCCI engine fed with n-heptane (diesel surrogate). The result proved that the solver provides stable simulations for all considered fuel blends/mechanisms. Simulation times with multi-component mechanism of NH_3, H_2 and n-heptane are on average 32 seconds per cycle with the solver reaching convergence after 6 cycles. The optimization conducted to support the mechanism/solver feasibility study implies optimum performance can be obtained for 90% NH_3 to 10% H_2 blend ratio, at compression ratio of 20 with lambda value of 2. At optimal operating conditions, indicated mean effective pressure (IMEP) was almost 2.7 times higher, indicated thermal efficiency (I_{eff}) is few points higher, and likewise more fuel economical than the baseline HCCI operation with n-heptane. At the same time, all emission quantifiers of the NH_3/H_2 HCCI engine, including NOx, were significantly reduced, while keeping the intrinsic advantages of zero-carbon fuel. Finally, it was concluded that the kinetic solver posed great potentials in aiding the HCCI technological advancement, also with the use of NH_3 and H_2 fuel towards a zero-carbon emission transportation system.

Notations

NH_3	Ammonia
H_2	Hydrogen
λ	Lambda
CA50	Crank angle at 50% heat release
ATDC	After top dead center
w/w%	weight by weight percent
BR	Blending ratio
CR	Compression ratio
ER	Equivalence ratio
IMEP	Indicated mean effective pressure
I_{eff}	Indicated thermal efficiency
ISFC	Indicated specific fuel consumption
CHR	Cumulative heat release
HRR	Heat release rate
MFR	Mass flow rate
AFR	Air to fuel ratio

1. Introduction

Traditional internal combustion engines (ICE) powered with fossil fuels as its main energy source, has been in use both in power generation and transportation sectors for centuries. However, they have been investigated to produce emissions (including nitrogen oxides NOx, hydrocarbon HC, carbon monoxide CO, and particulate

matter PM) which had negative impact on both public health and the environment [1]. Hydrogen (H_2) is among the viable option for the replacement of fossil fuels due to its renewable form, higher energy potential and lower ignition temperature [2]. However, due to its high volatility, storage and handling of H_2 is challenging, therefore raising debates of its employability in passenger and other transport vehicle [2]. Ammonia (NH_3, also from renewable sources) on the other hand, is less volatile and even has a higher energy capacity than H_2 [3]. It offers promising alternative fuel in terms of handling, energy density and safety. However, NH_3 is poor in combustion due to its high ignition temperature and low flammability (resulting from a slow chemical kinetics in the combustion process). These opposite characteristics of both fuels make them a perfect pair as H_2 may be used to enhance the auto-ignition property of ammonia in the NH_3/H_2 fuel blend [3].

Due to the advent of more environmental and health friendly options of fuel sources (such as biofuels), ICE optimization to accommodate these newly identified fuel types has led to the progressive research on more efficient combustion concepts [4]. Prospective routes for emission control includes the low-temperature combustion (LTC) enabling alternative fuel source. One option of LTC concept, the homogenous charge compression ignition (HCCI) combustion, has evolved in tandem with biofuel research. HCCI engines combines both elements of spark ignition (SI) and compression ignition (CI) engines. Air-fuel mixture is homogenously mixed before entering combustion chamber (as in SI engine) but ignition occur through compression instead of spark plugs (as in CI engines) [5]. In HCCI combustion mode, ignition is not instigated externally but by compression and autoignition of the air-fuel mixture. Ignition happens when thermodynamic conditions (temperature, pressure, specie concentrations) of the fuel are favorable [6]. This concept allows HCCI the use of different fuels (including biofuels, gasoline, diesel, both neat fuels and fuel blends) and their diverse physicochemical properties to regulate air-fuel autoignition and provides optimized engine operation over a wide range of operating conditions. These fuel flexibility properties of HCCI have prospects to contribute to energy security [7]. LTC and more homogenous mixing of fuel-air, has been investigated to also enable increase in engine performance metrics and a reduction of the emissions generated compared to traditional SI and CI engines. Challenges associated with the HCCI concept includes achieving a consistent combustion and controlling ignition timing under diverse operating conditions [5]. Research to address these challenges are ongoing for a more widespread use of the technology.

In engine performance optimization, the use of fast simulation models may be employed to enable rapid prototyping of robust engine models due to their high comparability [8]. Thereby, enabling applied level engine studies such as optimizing the operating limits of the engine design concept for technology development. HCCI simulation approaches, depending on run-time constraint application, range from Zero-Dimensional (0D) models, to high fidelity 3D models, with detailed Navier-Stokes equations solved using Computational Fluid Dynamics (CFD) [8]. 0D models are typically second law based, and order of magnitude faster than CFD. Fluid motion can be captured phenomenologically by dividing the volume to quasi-dimensional zones (that is, from single to multi-zone models depending on the order of complexity) [8]. Regardless of model fidelity, chemical kinetics is typically employed to simulate HCCI combustion progress. This reflects the reaction-driven nature of the phenomena and to capture ignition properties and combustion characteristics [5].

To address LTC development needs, chemical kinetic solvers have been recently included in the commercial engine simulation toolchains like GT-Suite (v2022 onwards) [9]. The applicability had not been thoroughly tested, especially when less-conventional fuel options are considered. To this end, using a n-heptane fueled single cylinder HCCI engine, Guo et al. [10] compared their experimental measurement with numerical simulations. They observed slight discrepancies in the heat release rate (HRR), in-cylinder pressure and other combustion parameter. This was predicted to be caused by the imperfect assumption of air/fuel homogenous mixing, combustion chamber wall temperature, reaction rates, uniform temperature and pressure, and also the fuel chemistry (level of detail of the applied chemical reaction mechanism applied in modeling). This led to the increment of the inlet temperature by 30 K for modeling HCCI, as recommended by Yelvington et al. [11]. They proposed that the use of 333 K as inlet temperature for the modeled case will allow a reduction in the deviation of the HRR phasing between both experimental and numerical modeling result data.

This study addresses the feasibility of kinetic solvers included in the GT-Suite, for the predictive combustion modeling of HCCI engine with multi-component fuel blend (consisting predominantly of NH_3 and H_2). This has not been publicly reported till date. To this end a baseline model with a suitable multi-component mechanism is validated over the experimental data available in the previously mentioned study by Guo et al. [10]. The validated model is further extended with H_2 and NH_3 injectors and benchmarked for combustion and emission performance over a wide range of operating conditions. Simulation convergence study and multi-parameter optimization complete the feasibility study and provide extended insight into the development concerns of advanced, multi-fuel combustion concepts.

2. Methods

2.1 Setting up the HCCI engine model, including engine specifications, geometry, and boundary conditions

For the HCCI model setup, a 1-cylinder HCCI engine (fueled with n-heptane) was selected from GT-Suite template [12]. This baseline model was calibrated using engine specifications from the single cylinder HCCI engine experiment conducted by Guo et al. [10]. Table 1 has presented the HCCI engine models (both baseline and present study) specifications, geometry, and other initial conditions. For the purpose of this study, a dual fuel 1-cylinder HCCI engine was modeled. NH_3 and H_2 were the target fuels. The InjRateConn injector type was used to introduce the H_2 fuel into the engine model for present study. Engine model specification included standard SI injection timing and valve timing. Combustion object used in the engine cylinder is the EngCylCombHCCI. This object called the EngCylChemGas object to define both the gaseous reaction mechanism and the thermodynamic fluid properties from external files. This automatically created all necessary FluidNASA-LiqGas fluid species reference objects needed for the chemical reaction mechanism. Details on selected chemical reaction mechanism development and validation has been included in subsection 2.2. Combustion was assumed to be truly homogenous. The cylinder Initial state object has been defined by object value “Init-FA”, which was used to impose boundary conditions such as absolute pressure, fluid temperature and composition at the start of the simulation. Value for both absolute pressure and temperature have been listed in Table 1. The initial fluid composition defined with the object value “FA-Mixture”, which called fluid object “air”, “NH_3” and “H_2” with specified mass fraction as 0.95, 0.04 and 0.01 respectively. For the n-heptane fueled HCCI model, the object value “FA-Mixture” called fluid object “air”, and “NC_7H_{16}” with specified mass fraction as 0.95 and 0.05 respectively. Exhaust gas recirculation (EGR) intake fraction set to 0.2. Cylinder wall temperature defined by object value “TWall”, which defined the head and piston temperature as 575K, and the cylinder temperature as 400K. This represented the temperature of the wall surface directly in contact with the fluid. The heat transfer properties in the cylinder defined by object value “Woshni”. This presented the heat transfer model as WoshniGT, overall convection multiplier as 1, head/bore area ratio as 1.3, piston/bore area ratio as 1.03, convection temperature evaluation as hybrid, and enabled the low speed heat transfer enhancement for the heat transfer model. Start of cycle was at -144 ^oCA at intake valve closing and exhaust valve closing at 140 ^oCA, replicating the experimental valve timing from Guo et al [10].

Table 1. HCCI engine model specifications, geometry, and operating conditions

Item	Baseline single-fueled HCCI model (experiment)	Dual-fueled HCCI engine (GT-suite)
Engine specification and geometry	1-cylinder, four stroke HCCI, bore =82.55mm, Stroke = 114.3mm, displacement=0.6117L, connecting rod length = 254mm, intake valve close (IVC) = -144 ^oCA, Exhaust valve open (EVO) = 140 ^oCA, EGR = 20%	
Boundary conditions	Temperature = 303 K, Pressure = 95 kPa	Temperature = 333 K, Pressure = 100 kPa
Target fuels	n-Heptane	NH_3/H_2 blend
No of injectors	1	2
Total fuel energy (TFE)	67,6 MJ	67,6 MJ

2.2 Chemical kinetics mechanism selection

A reduced chemical kinetic mechanism developed by Patel et al. [13] was used for the baseline model simulation. The reduced mechanism was generated starting from an existing n-heptane mechanism containing 165 reactions and 40 species. The reduced mechanism was generated using SENKIN to produce ignition delay and solution files, and XSENKPLOT to analyze the reduced reaction mechanism. The newly formulated and reduced reaction mechanism was then used to generate new ignition delay data. Finally, kinetic constants in the new mechanisms were adjusted to improve ignition delay and engine combustions to account for diesel fuel cetane number and composition. The newly-reduced mechanism consists of 29 species and 52 reactions, and was validated under constant volume engine conditions. In comparison with a comprehensive mechanism (having 179 species and 1642 reactions), the new reduced mechanism gives similar predictions. Reduced chemical reaction mechanism were often used to enhance the computational efficiency of engine simulations

[13]. Researchers have successfully applied the reduced mechanism developed by Patel et al. in HCCI concepts. Jia et al. [14] implemented an improved phenomenological soot model coupled with the reduced n-heptane chemical mechanism developed by Patel et al., into KIVA-3V code to describe soot formation and oxidation process in a n-heptane HCCI combustion. The model was validated both experimentally and computationally. The results demonstrated satisfactory accuracy on all the studied parameters [14].

For the NH_3/H_2 fueled HCCI model, a detailed chemical kinetic mechanism and thermodynamics data file developed by Stagni et al. [15] for low temperature combustion was used for model simulation. Stagni et al. investigated the oxidation of NH_3/H_2 blends under low and intermediate temperature conditions using experimental methods in a flow reactor at near atmospheric pressure of 126.7 kPa and using stoichiometric conditions. They also developed a comprehensive kinetic model to interpret the experimental results. Fuel conversion and autoignition at low temperature were confirmed for the fuel blend with a reactivity boost provided by the addition of H_2. The kinetic mechanism contained 203 reactions and 31 species. This included a comprehensive list of species involved in the NH_3 reaction, including all radicals, intermediates and products. Table 2 presents both fuel type kinetic mechanisms to help understand model fidelity. NH_3/H_2 reaction mechanism has also been validated by Xu et al. [16]. The validation was carried out by comparing the results obtained from the mechanism with experimental data. The laminar flame speeds were calculated using CHEMKIN-PRO software with the developed mechanism. The calculated flame speeds were then compared with experimental results obtained by Han et al. [17]. The comparison of these results under different hydrogen content at room temperature and atmospheric pressure demonstrated that the chemical mechanism is reasonable for stimulating the overall combustion rate of NH_3/H_2/air mixtures in HCCI concepts.

Table 2. Chemical reaction mechanism selection based on target fuel and deired level of detail

Primary surrogate	Source	No of species	No of reactions	NOx mechanism
n-Heptane	Patel, A., Kong, S., and Reitz, R. [13]	29	52	*NA
NH_3/H_2	Stagni et al. [15]	31	203	Zeldovich -based

*refers to not applicable

2.3. Baseline model validation

To validate the applicability of the baseline model, the operating conditions used for the HCCI engine experiment by Guo et al. [10] was used in GT-power simulation. The experiment was conducted in a single cylinder co-operative fuel research (CFR) engine modified and equipped with an air assist port fuel injector, similar to the single cylinder HCCI baseline model in GT-power. Boundary conditions for the simulation were set in accordance to experimental reference, as follows; Compression Ratio (CR) as 10, intake temperature as 303K, intake pressure as 95 kPa, AFR as 50 and engine speed as 900 rpm. The experiment was tailored towards capturing the n-heptane fueled HCCI engine performance and combustion characteristics at individual parameter sweeps (engine speed and CR particularly). Combustion parameters such as CA50 (crank angle at 50% heat release), IMEP, ISFC, and COVIMEP (coefficient of variation of indicated mean effective pressure) were monitored continuously in four tests to ensure accurate data collection and analysis.

For reproducing this HCCI engine model validation in GT-power, adjustment was made to the intake fluid mixture temperature by an increment of +30 as proposed by Yelvington et al. [12]. This correction was applied to all operating conditions. On this basis, the model was able to replicate the effect of CR and engine speed on the combustion phasing (CA50). The in-cylinder peak pressure and the CA50 measured data from the model were also validated against the experimental data from Guo et al. Results of the validation has been presented in subsection 3.1. This simulation study only considered the results obtained from combustion between IVC and EVO.

2.4. Scope of the research

Upon completion of model validation, a second injector was added for delivering H_2 fuel to the engine model. Simulations were run to investigate the effect of fuel blending ratio (BR), air-to-fuel ratio equivalence (ER), CR, and engine speed, on the performance, emission and combustion characteristics of an NH_3/ H_2-fueled HCCI engine in comparison with heptane-fueled HCCI engine model. The selected range of engine operating condition for parametric sweep were as presented in the baseline experimental study. Total fuel energy (TFE) introduced into the new model was kept constant at 67.6 MJ, equating the amount of fuel energy introduced for the baseline model, to enable effective comparison of their results. Table 3 presents the BR for NH_3/H_2 from pure NH_3 (NH_3/100) to 50% NH_3 to H_2 blend (NH_3/50), as a function of their mass flow rate (MFR) and lower heating value (LHV). Based on the initial sweeps, range of

operating conditions were refined for further optimization. Parametric sweeps study was done choosing appropriate range and step-size for each parameter. The simulation matrix is presented in Table 4. The results on engine performance metrics and combustion phasing observed as a function of the parametric sweeps. Optimal operating conditions that achieved desired results were selected for iterative refinement. Optimization was realized by fine-tuning the operating conditions to converge towards optimal engine performance, combustion phasing and emissions. Final optimization was made with simulation test 5 as seen in Table 4.

Table 3. Blending ratio (BR) for NH_3/H_2 fueled 1-cylinder HCCI engines. *LHV_H_2 = 120 MJ/g, *LHV_NH_3 = 18.8 MJ/g. *Data from Lhuillier et al. [18]

BR (w/w%) (NH_3/H_2)	100/0	90/10	80/20	70/30	60/40	50/50
MFR_H_2 (g/s)	0	0.23	0.35	0.41	0.46	0.49
MFR_NH_3 (g/s)	2.70	2.10	1.39	0.96	0.69	0.48

Table 4. Simulation matrix for NH_3/H_2 fueled 4-cylinder HCCI engines. Inlet temperature=333K, Inlet pressure=1bar

Simulation test	Speed (rpm)	CR	ER (λ)	BR (w/w%) (NH_3/H_2)
1	900 – 4500	20	1	90/10
2	3500	16 – 24	1	90/10
3	3500	20	0.8 – 3	90/10
4	3500	20	2	50/50 –100/0
5	3500	20	1-2	90/10

Fuel-air mixture is among the several causes that may contribute to cycle to cycle variability (CCV). The ER parametric sweep was used in the final optimization in order to achieve optimum solutions. This variability impact combustion timing, maximum pressure and heat release rate. CCV analysis was done by creating scatter plot of CA02/CA50 for all cycles, at selected engine operational point. Results of CCV are presented in subsection 3.3. To run the above case setup, simulation time control was set to periodic, simulation duration was also set to 6 cycles, and in the initialization tab, previous case was set to help the simulation converge faster. HCCI model simulation was initialized and then redirected to GT-Post (an interface for postprocessing and analyzing result data on GT-Power). 5 sets of simulation test were carried out, with test 1 to 4 as main simulation and test 5 as a rerun optimization.

3. Results

3.1 Baseline Model validation results

According to Fig. 1, GT-power was able to reproduce the experiment results discussed in section 2.3, better while using the proposed simulation temperature 333K. The model was able to capture the combustion phasing in line to the experimental reference, while keeping the same combustion efficiency. CA50 predictions closely matched the experiment at zero-degree ATDC. In-cylinder maximum pressure was adequately reproduced, showing that simulated model reaction pathways were well represented. A difference of 0.5bar may be associated to random errors from the experiments. Low temperature reaction (LTR) predicted to occur earlier in the simulation than in the experiment. Likewise, there was an observable sharp rise in the heat release rate (HRR) at CA50 from the simulated model compare to the experiment. Both over-estimations result primarily from neglects of thermal stratification in 0D, single volume approach. Multizone models are typically able to capture the stratification much better as the kinetic solution progresses slower in the colder zones near the cylinder boundary [19]. The difference is also associated to inaccuracies in determining the boundary conditions on the engine airpath [20] and shortcomings of the incorporated mechanism itself [21]. The mechanism used in this baseline study was generic. Although, the reduced mechanism by Patel et al. was validated on a reference CFR engine, and widely incorporated in various HCCI studies using N-heptane as surrogate.

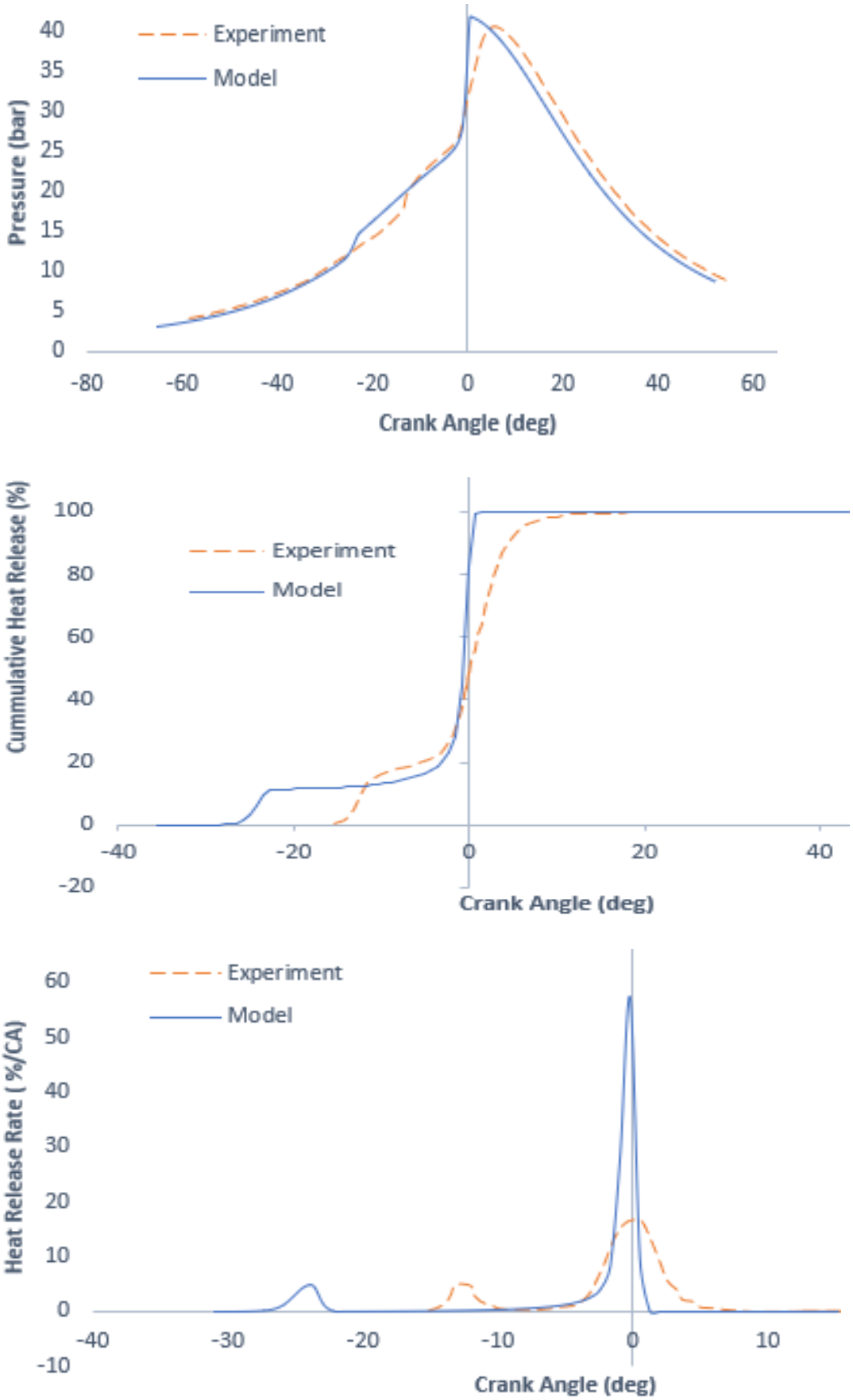

Fig 1. Comparison of simulated model (top) in-cylinder pressure (middle) cumulative heat release (bottom) Heat release rate, against the experimental data. AFR=50, CR=10, Intake pressure = 95 kPa.

HCCI is very sensitive to IVC conditions including residual gas temperature and composition, exact fuel make-up (including impurities) and secondary on the thermal in-cylinder stratification. Neither of these parameters were directly available for the baseline engine used in this study and the model calculated the IVC conditions starting from simplified data on the port geometry and valve timing information.

The scope of the research did not deem fit re-tuning the mechanism for this particular experiment (commonly done by studies that show exact HRR match) as this brings bigger risk of over-constraining the predictive features of the model. The approach is considered proper considering the main goal of the study – assessing the functionality for GT-Suite kinetic solver in fast engine simulations. As such, the only tuning parameter was the cylinder-area averaged wall temperature which was not explicitly known from the experiments and used to target the reference CA50. Considering the fidelity of the approach, the resulting performance parameter estimation (main use case of 0/1-D engine models) are more than satisfying, as Pmax, IMEP and engine efficiency are predicted well.

CA10 or CA90 are on the other side, very difficult to predict for HCCI in a computationally efficient 0-D combustion model. This is related to the fact that spatial temperature inhomogeneity is not captured [19]. The model captures the correct trends in this respect, confirming predictivity. On the other hand, CA10 in HCCI is determined majorly by the pre-ignition reactions that do not contribute significantly to the performance and emission formation. The efficiency in HCCI is shaped predominantly by correct combustion onset (CA50) and the amount of energy released due to incomplete combustion. Both of these parameters are captured correctly considering the CHR plots in Fig. 1. As such we consider this model suitable for computationally efficient pre-design, pre-optimisation or control design studies as further substantiated by main body of the result discussion. Table 5 also presents a comparison of baseline experiment versus simulation results of the CA10, CA50 and cylinder maximum pressure.

Table 5. Comparison of baseline HCCI engine combustion experiment results (Guo, et al., 2010) versus GT-power model simulation (present study)

Test	CA10 (ATDC)	CA50 (ATDC)	Maximum Pressure (bar)
Experiment	-12.5	0	42.5
GT-power simulation model (333 K)	-21.5	0	42.0

The model is able to capture the effect of varying engine speed on CA50, similarly to the experimental data as seen in Figure 2.

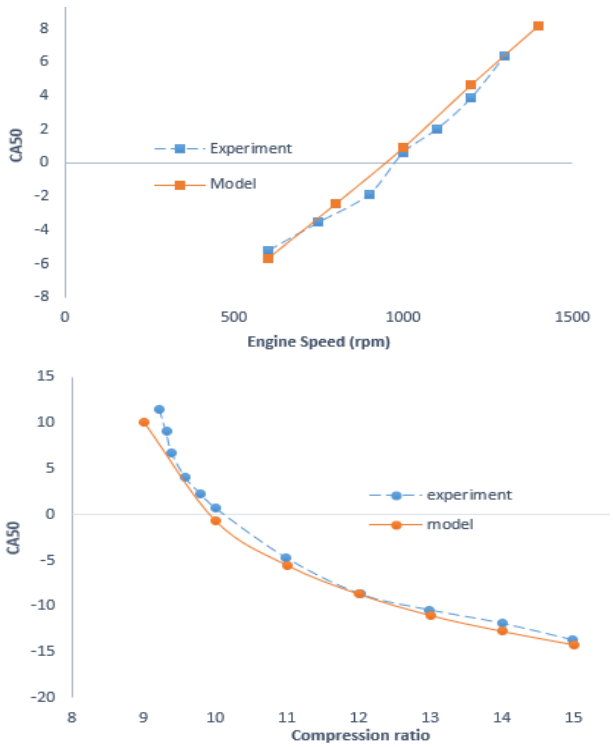

Fig. 2. Comparison of experimental CA50 (top) against engine speed, and (bottom) against CR, against GT-power model simulation results. AFR =50, CR=10, P=95 kPa

Simulated engine speed varied from 600 rpm to 1500 rpm and 333K. Resulting data points from the simulated model were almost linear, while those of the experiments showed some deviations even though the trends in both were coherent. CA50 was observed to increase as the engine speed increased, which is understandable as the kinetic timescale of the combustion commences under faster resolving in-cylinder volume. At 900 rpm, CA50 was at zero-degree CA, ATDC. Effect of varying CR on CA50 is further shown in Fig. 2. The observed decrease in CA50 with increased CR, is attributed to shorter combustion duration since kinetically controlled combustion process is faster in this condition [10]. Importantly, both the simulated and experimental trends were coherent. Individual resulting data points were almost corresponding for all cases and error were very minute. Simulation error in CA50 did not exceed 1.5CA for either of the operating points in Fig. 2. Taking to account the above discussion, the predictivity of the modeling framework is considered validated in terms of HCCI phenomenology. Consequently, the model can be further used for extrapolating the combustion concept towards NH_3/H_2 fueling, under constraints of the validity of the kinetic mechanism involved.

3.2 Analyzing Combustion parameters and performance metrics of NH_3/H_2 fueled HCCI engine

3.2.1 Effect of varying engine speed on NH_3/H_2 combustion

Simulation test 1 was carried out at inlet conditions of 333 K and 1 bar, and at a constant TFE of 67.6 MJ. As NH_3 does not burn readily in its pure form, initial BR used for the simulation was NH_3 (90%) (i.e. with 10 w/w% H_2). For initial test, CR was set to 20 and engine speed varied from 900 rpm to 3500 rpm. At baseline engine speed of 900 rpm, engine performance and combustion parameters were poor as presented in Table 6 and Fig. 3 respectively. However, between 2000 rpm to 3500 rpm, there was stable combustion. At engine speed higher than 3600 rpm, there was loss of convergence in the simulation. This was perhaps indicative of the range of engine speed upon which the engine can operate, based on the engine specifications and the boundary conditions. Indicated mean effective pressure (IMEP) and indicated thermal efficiency (I_{eff}) increased with increasing engine speed. Indicated specific fuel consumption (ISFC) stabilized between 2500 rpm to 3500 rpm as presented in Table 6. In-cylinder pressure (Pmax) also increased with increase in engine speed. This may result from the accumulated heat during compression stroke because of shorter cyclic period as discussed by Hasan et al. [21]. Additionally, with increasing speed, the cumulative heat release (CHR) improved and combustion phasing advanced as illustrated in Fig. 3. This test proved engine speed as an important parameter with significant effect on the combustion and performance of HCCI engines.

Table 6. Engine performance metrics for varying engine speed from 900 rpm to 3500 rpm, ER=1, BR=NH_3(90%), P=1 bar, T=333K

Engine Speed (rpm)	900	1500	2000	2500	3000	3500
IMEP (bar)	0.6	2.75	5.15	6.59	7.75	8.32
I_{eff} (%)	1.00	7.04	15.99	23.22	28.23	31.44
ISFC (g/kW-h)	3166.86	600.48	346.82	295.7	305.3	310.54

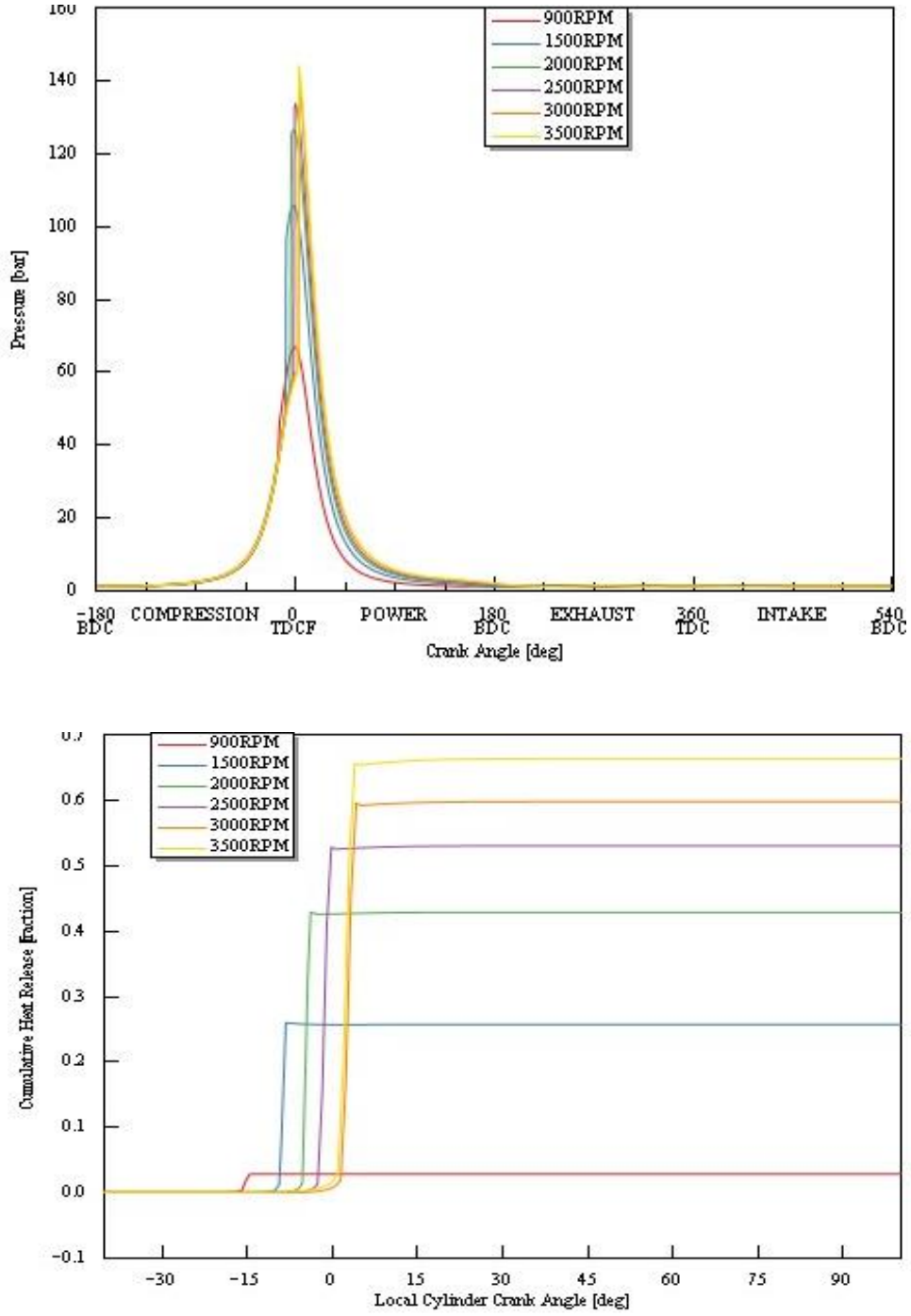

Fig. 3. Combustion parameter plots for NH_3/H_2 fueled HCCI engine over varying engine speed, (top) In-cylinder Pressure (bottom) Cumulative heat release. Varying engine speed from 900 rpm to 3500 rpm, ER=1, BR=NH_3(90%), P=1 bar, T=333K

3.2.2. Effect of varying compression ratio on NH_3/H_2 combustion

Simulation test 2 was executed with a CR case sweep range of 16 to 24 and incremental step of 2. BR was fixed at NH_3 (90%), ER of 1, engine speed of 3500 rpm, inlet temperature and pressure as 333K and 1 bar respectively. At this operating conditions, CR of 22 and 24 proved to be too high and caused excessive Pmax as illustrated in Fig. 4. This trend presents the effect of CR on the combustion characteristics. I_{eff} should conventionally increase with CR. However, here opposite trend is observed. This is mainly because CA50 is unoptimized, occurring nearly 10^0 CA before TDC. Excessively high in-cylinder pressure can be detrimental to the engine overall efficiency over time. Engine performance

metrics were also better at lower CR of 18 and 20 presented in Table 7. Although CR less than 18 gave rise to an unstable combustion where all engine performance were all negative. This implied that at CR lower than 18, compression pressure was not enough for the autoignition of the air-fuel mixture and the thermodynamic conditions were not favorable [6].

Table 7. Engine performance metrics for varying CR at constant engine speed=3500 rpm, ER=1, BR=NH_3(90%), P=1 bar, T=333K

CR	16	18	20	22	24
IMEP (bar)	-	8.35	7.93	7.80	7.43
I_{eff} (%)	-	31.66	30.75	30.01	28.55
ISFC (g/kW-h)	-	308.68	316.69	320.42	337.37

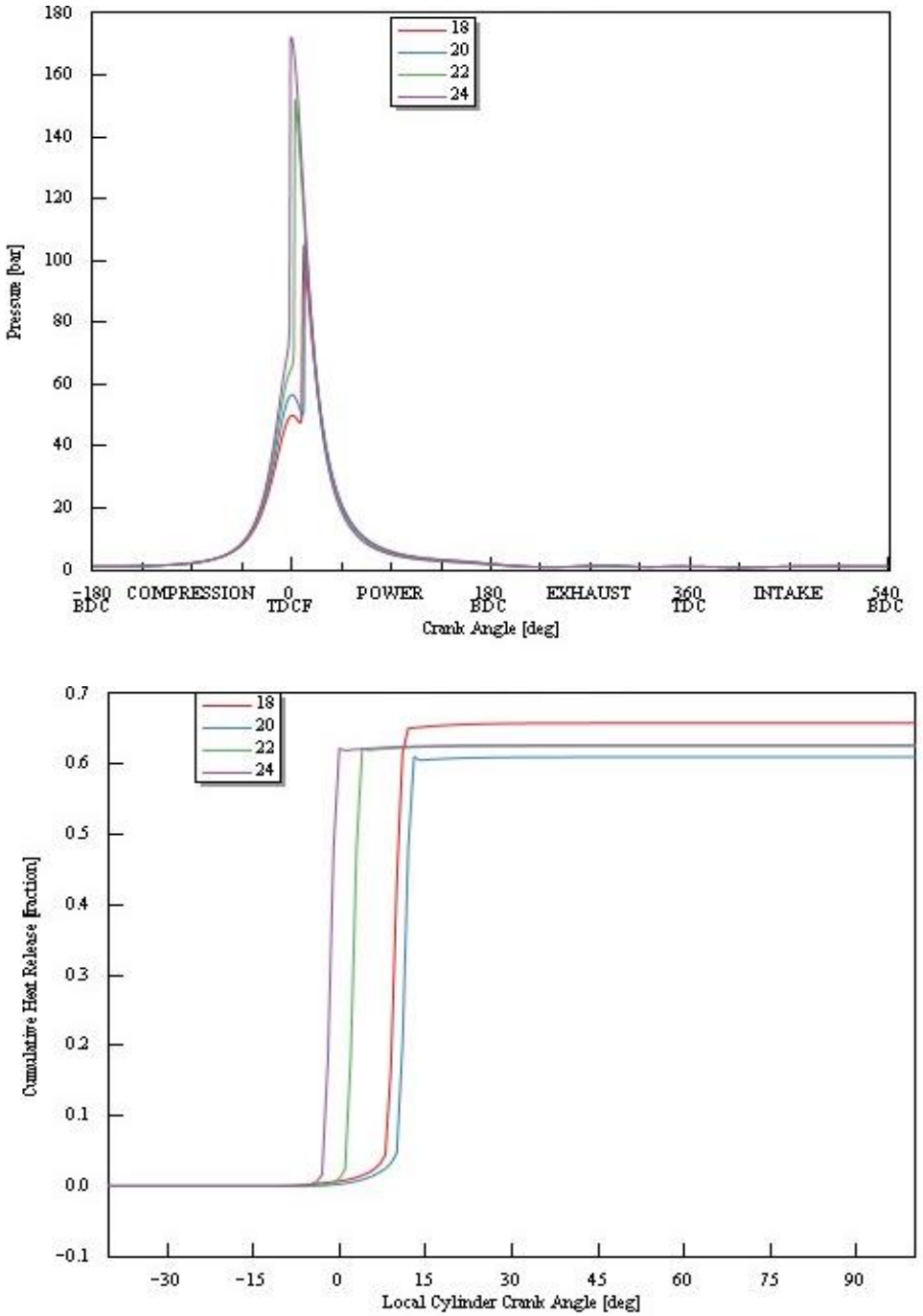

Fig. 4. Combustion parameter plots for NH_3/H_2 fueled HCCI engine over varying CR, (top) in-cylinder pressure, (bottom) Cumulative heat release. Constant engine speed=3500 rpm, ER=1, BR=NH_3(90%), P=1 bar, T=333K

3.2.3. Effect of varying equivalence ratio on NH_3/H_2 combustion

At fixed TFE of 67,6 MJ, CR at 20, engine speed at 3500 rpm, inlet temperature and pressure as 333 K and 1 bar respectively, the effect of varying ER on the HCCI combustion of NH_3 (90%) was investigated. ER (Lambda) was used to quantify the actual air to fuel ratio relative to the stoichiometry required to achieve complete combustion. From the fuel injector introducing NH_3 into the engine model, the air to fuel ratio was defined as lambda. This lambda was then varied as a parameter. Simulation test 3 was done with ER case sweep range of 0.8 to 3. ER of 0.8 indicated a rich mixture, while ER of 3 indicated a very lean mixture. Fig. 5 presents the effect of varying ER on Pmax and CHR. Combustion delayed with decrease in lambda. This phenomena was natural as the fuel molecules requires enough air molecules for complete combustion chemistry. At lambda value 0.8 indicating a rich mixture, CHR was lowest, ISFC was highest and, the overall engine thermal efficiency was lowest. Although, 1 is the standard lambda value however optimal CHR, ISFC, and the best thermal efficiency was observed at lambda value 2 for the set operating conditions as illustrates in Table 8. Likewise, combustion phasing parameter CA50, presented better at very lean mixture of lambda 2. The fuel blend might require more air than stoichiometry for better phasing of a complete combustion.

Table 8. Engine performance metrics for varying ER at constant engine speed=3500 rpm, CR=20, BR=NH_3(90%), P=1bar, T=333K

ER (lambda)	0.8	1	1.5	2	2.5	3
IMEP (bar)	7.97	8.40	8.41	8.38	7.47	6.85
I_{eff} (%)	26.69	31.09	38.94	42.94	40.68	38.69
ISFC (g/kW-h)	408.19	325.68	196.05	149.10	137.25	131.37

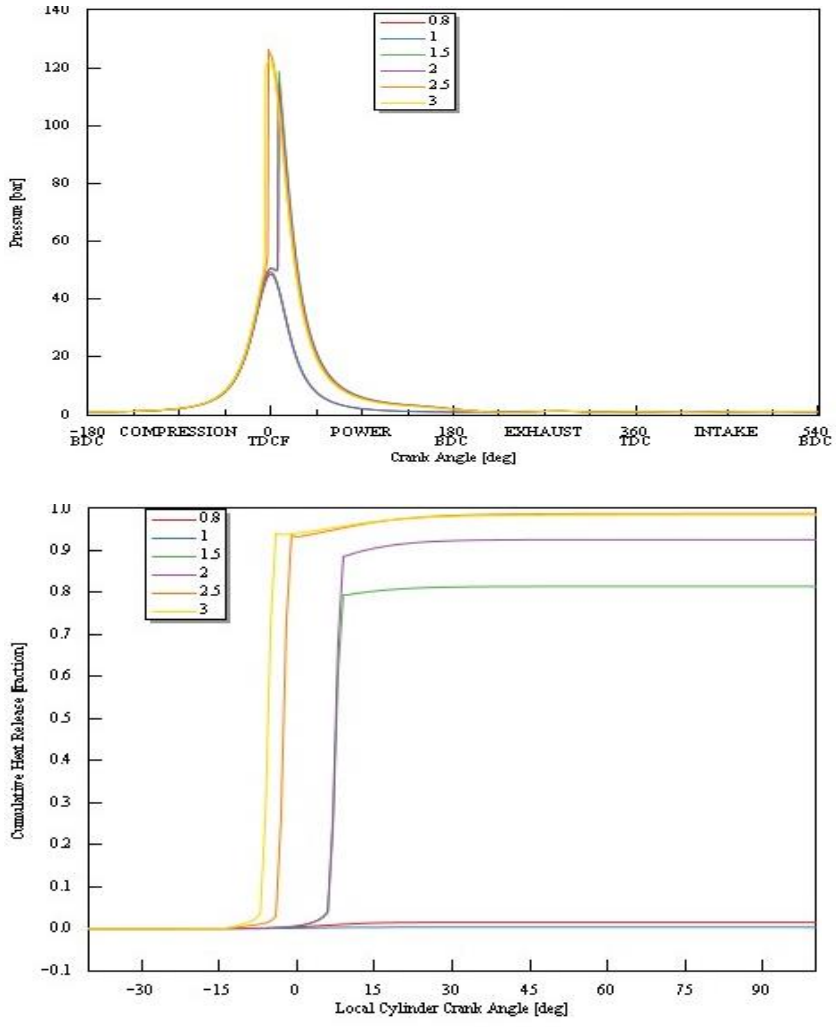

Fig. 5. Combustion parameter plots for NH_3/H_2 fueled HCCI engine over varying ER, (top) in-cylinder pressure, (bottom) Cumulative heat release. Constant engine speed=3500 rpm, CR=20, BR=NH_3(90%), P=1bar, T=333K

3.2.4. Effect of varying fuel blending ratio on NH_3/H_2 combustion

Table 9 and Figure 6 represents the effect of BR on the HCCI combustion and performance for fixed TFE of 67,6 MJ. For CR at 20, engine speed at 3500 rpm, ER of 2, inlet temperature and pressure as 333 K and 1 bar respectively, simulation test was performed for NH_3/H_2 BR of 100/0, 90/10, 80/20, 70/30, 60/40, and 50/50. Table 5 already presented the BRs for NH_3/H_2 from pure NH_3 to NH_3 (50%), as a function of their MFR and LHV. This is to allow for clear presentation of results. Pure NH_3 did not combust readily in the engine model as illustrated on the CHR in Figure 6. Pmax at this operating conditions was relatively same for all BR except pure NH_3. Engine combustion and performance metrics were optimal at BR of 90. The CHR graph illustrated that, the more H_2 fraction in the fuel blend, the earlier combustion was initiated. However, CHR was highest in the fuel blend with the lowest H_2 fraction. The effect of the BR can also be seen engine efficiency, as BR of 90 presented the highest I_{eff} and IMEP. This phenomena portrays that H_2 was good for improving the ignition properties of NH_3. However, heat of combustion of NH_3 was above 1.3 times that of H_2 fuel [22]. This was reflective from the CHR values for the various BR. An increase in the NH_3 percentage fraction from 80 to 90 in the fuel blend, resulted into almost about 30% increase in the cumulative heat release.

Table 9. Engine performance metrics for varying BR at constant engine speed=3500 rpm, ER=2, CR=20, P=1bar, T=333 K

BR (NH_3/H_2)	100/0	90/10	80/20	70/30	60/40	50/50
IMEP (bar)	-0.5	8.23	7.38	6.89	6.42	6.06
I_{eff} (%)	-3.4	40.19	28.01	23.01	19.53	17.57
ISFC (g/kW-h)	0	173.23	168.24	184.55	205.06	219.02

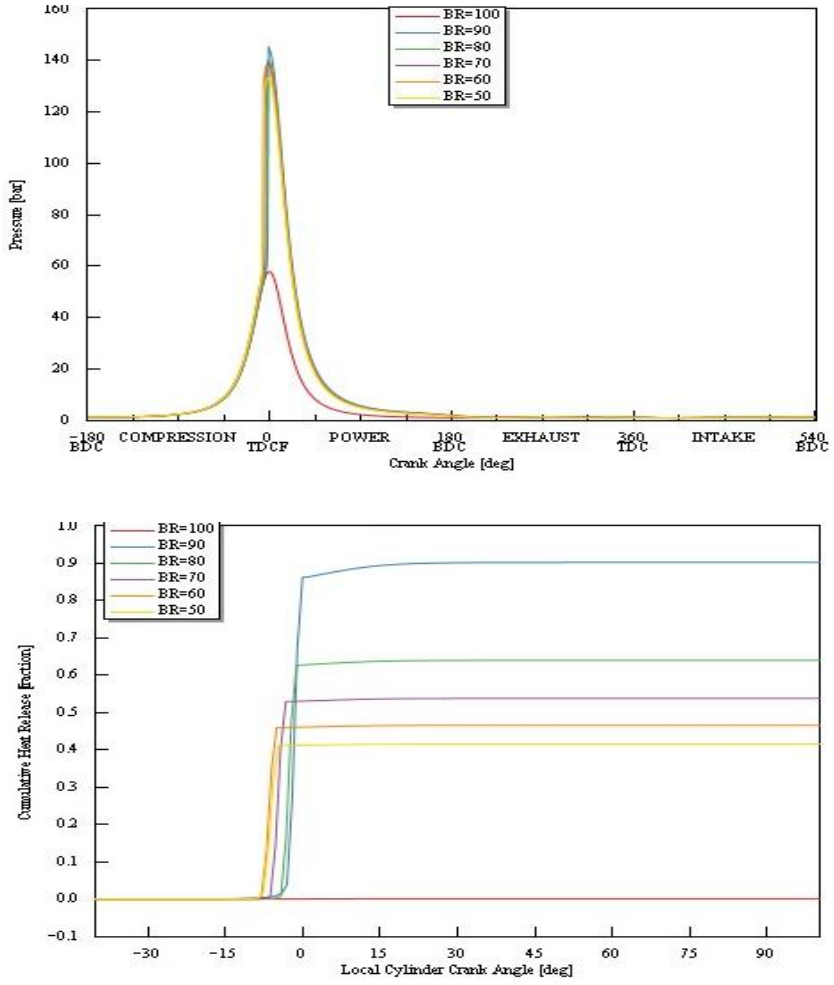

Fig. 6. Combustion parameter plots for NH_3/H_2 fueled HCCI engine over varying BR, (top) in-cylinder pressure, (bottom) cumulative heat release. Varying BR at constant engine speed=3500 rpm, ER=2, CR=20, P=1bar, T=333K

3.2.5. Final round optimization on NH_3/H_2 combustion engine.

A combination of operating conditions producing optimal engine performance and combustion phasing was used for the simulation of the final round optimization. At fixed engine speed of 3500 rpm, CR of 20, TFE of 67.6 MJ, BR of NH_3/H_2 as 90/10, inlet temperature and pressure as 333 K and 1 bar respectively, ER was varied between 1 and 2 to compare combustion of stoichiometry mixture, to lean mixture. Table 10 shows that with ER of value 2, engine performance metrics are better. Fig. 7 presents that there was a 35% higher CHR at ER of 2 than 1. This illustrated that there was higher heat of combustion at ER of 2. Although there was zero carbon emissions from both cases, however, NOx emission level was higher at ER value of 2. This might be due to more oxygen radicals forming more bonds with the available nitrogen, as a result of the excess air to fuel ratio from ER value 1 to 1.5 and to 2. This was where the tradeoff occurs. It presents a situation of making a choice between engine overall efficiency or the engine NOx emissions.

Table 10. Engine performance and Combustion metric from final round optimization. Engine speed=3500 rpm, CR=20, P=1 bar, T=333 K, BR=NH_3(90%)

ER	IMEP (bar)	I_{eff} (%)	ISFC (g/kW-h)	Pmax (bar)	Tmax (K)	CA50 (deg)	NOx (ppm_emissions)	HC (g/kW-h)	CO, CO2 (g/kW-h)
1	8.2	30.8	318.6	143.5	2702	1.7	42.4	0.19	-
1.5	8.4	38.9	196.1	137.6	2818	4.6	180.7	0.07	-
2	8.4	42.9	149.8	144.2	2896	0.5	1045.5	0.00	-

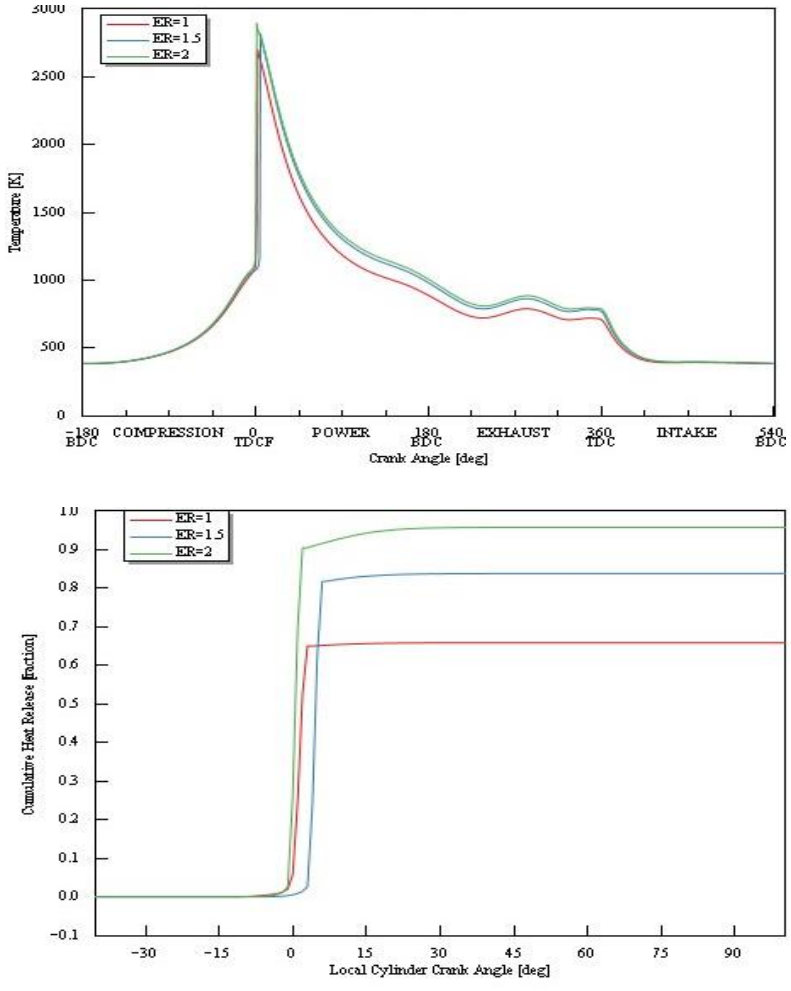

Fig. 7. Combustion parameter plots for NH_3/H_2 fueled HCCI engine over varying ER, (left) cylinder max temperature (right) cumulative heat release. Engine speed=3500 rpm, CR=20, P=1 bar, T=333 K, BR=NH_3(90%)

3.3. Cyclic variability and engine comparability.

For ensuring stability and reliability of the results, a cycle-to-cycle variability analysis performed for both the current study engine model and the baseline model. The CA02 (crank angle at 2% total heat release) and CA50 investigated against the cycle numbers as illustrated in Fig. 8. This was significant for understanding the combustion stability and assessing how efficiently the fuel combustion is proceeding. The combustion in the baseline model already became stable at cycle number 3 and continued to remain stable for the rest of the cycles. Although combustion phasing was unstable during the first four cycles in the NH_3/H_2 engine model, however phasing became stable at cycle number 5 and retained stability until the end.

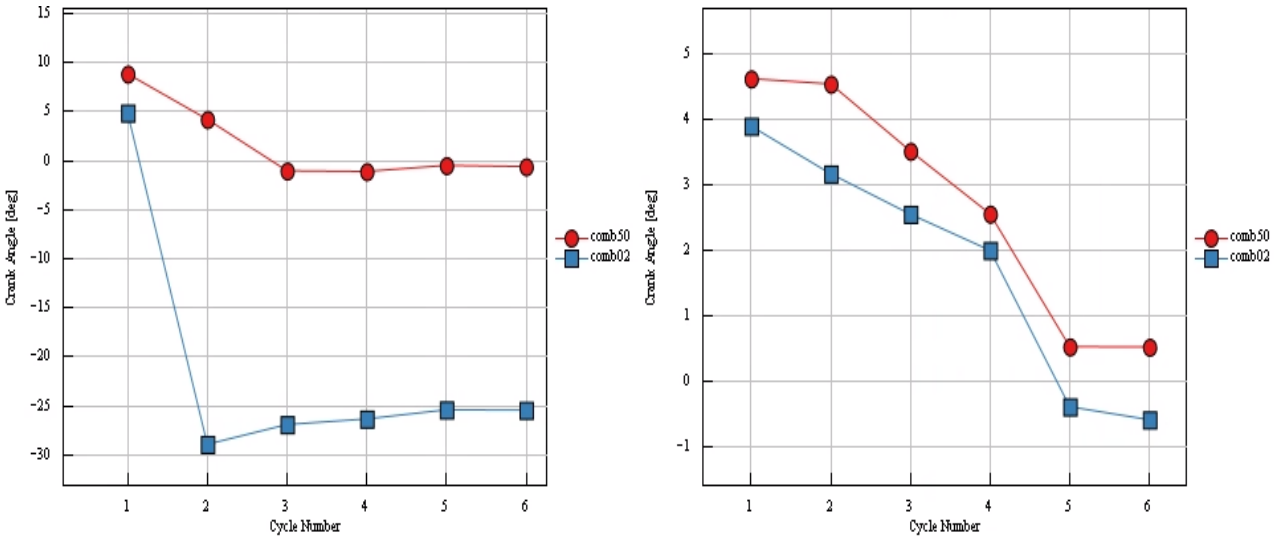

Fig. 8. Scatter plot for CA02/CA50 for all cycles in, (left) n-Heptane fueled engine model (right) NH_3/H_2 engine model.

4. Discussion

4.1 Summary of the simulation results and analysis of HCCI combustion behavior

This study investigated the effect of engine speed, NH_3/H_2 fuel BR, ER, and CR on the engine performance metrics, combustion phasing and emission characteristics. The study was initiated with BR ratio of 90%/10% for NH_3/H_2, respectively, ER of lambda value 1, and CR of 20. Engine speed was varied and observed as a crucial parameter, which significantly had effect on the combustion phasing and engine performance as illustrated in table 6 and Fig. 3. As engine speed increased, the timing of autoignition was better optimized, likewise the engine thermal efficiency and IMEP. The optimized engine speed was 3500 rpm while keeping other operating conditions constant. At engine speed higher than this, the simulation did not reach a convergence. The reason behind the NH_3/H_2 fueled HCCI engine, running at faster speed may be that the fuel blend had a faster combustion characteristic compared to heptane fuel. H_2 has a high flame speed and can contribute to the faster combustion [23], allowing quicker energy release and enabling the engine run efficiently at higher speeds than that of the n-heptane fueled engine model. The fuel reactivity could play a role in the influence on the engine speed. While keeping other operating conditions constant, CR was varied between 18 to 24. As CR increased, the combustion process advanced, and the peak in-cylinder pressure increased as illustrated in Fig. 4. This trend presented the effect of CR on the combustion characteristics. Although excessively high in-cylinder pressure was detrimental to the engine overall efficiency over time [24]. CR less than 18 gave rise to an unstable combustion where all engine performance were all negative. This implies that at CR lower than 18, compression pressure was not enough for the autoignition of the air-fuel mixture and the thermodynamic conditions were not favorable. Additionally, natural aspiration is considered for the engine operation, warranting higher CR. A value of 20 was observed for CR to be optimal for engine performance and combustion parameters.

The blending of NH_3 and H_2 fuel depends on specific applications and desired engine performance. Pure NH_3 misfired, but with as little as 10% H_2 in the fuel energy mix, auto-ignition occurred and

performance drastically improved as stated in Table 9 and Fig. 6. However, with increasing fraction of H_2 in the fuel blend, there was observable decrease in the cumulative heat release. This could be as a result of the combustion characteristic of H_2 fuel. H_2 has a faster combustion rate and wider flammability and as a result [24], an increase in the fuel blend fraction will shift the combustion characteristics towards that of H_2 which ignites faster but less intense combustion process. This caused CA50 to occur before TDC. It also resulted into an overall lower cumulative heat release as the fraction of H_2 increased in the blend. Dilution effect from fuel blend might also affect the overall kinetics and concentration of the reacting species, potentially causing a reduction in the heat release rate, as discussed by Oakley et al. [25] in their study.

The air to fuel ER also had significant effect on the overall engine performance, particularly on the emission characteristics. The heat release rate and cumulative heat release were also higher at a very lean air-fuel mixture, although combustion phasing remained almost at zero-degree crank angle. The intrinsic advantages of zero-carbon fuel was observed for all cases; however, NOx emission level was higher at ER value of 2. NOx Concentration was proportional to peak cylinder temperature. Among the three ER cases, ER of value 2 resulted into the highest in-cylinder temperature. Additionally, formation of more NOx might be due to more oxygen radicals forming more bonds with the available nitrogen as a result of the excess air to fuel ratio from ER value 1 to 1.5 and to 2, while having the best engine performance metric and overall efficiency at ER value as 2. This is where the tradeoff occurs. It presents a situation of making a choice between engine overall efficiency or the engine NOx emissions. This result is corresponding to the study of Meng et al. [26]. They concluded from their study that an increasing inlet pressure with a relatively high ER was favorable for NH_3 combustion, although a higher NO formation observed due to high activity of OH and HNO from the chemical kinetics behaviors.

A comparison summary of the performance metrics, combustion parameters and the emission characteristics of both modeled HCCI engines have presented in Table 10. Given the operating conditions as presented in the table, the NH_3/H_2 fueled engine enables a higher engine speed. IMEP was almost 2.7 times higher, indicated efficiency (I_{eff}) was few points higher, and likewise more fuel economical than baseline engine. Overall emission characteristics was also better than the baseline engine. Although NOx emissions was shown to be more, but very low as values as given in parts per million (ppm) emission. There might also be a high NOx from the baseline engine but the chemical reaction kinetics model used for the baseline engine model did not include a NOx mechanism as presented in Table 2.

Table 11. Engine performance and Combustion metric from comparison of the n-Heptane fueled HCCI versus NH_3/H_2 fueled HCCI engine. P=1 bar, T=333 K, ncyc = 6

Items	**n-Heptane**	**NH_3/H_2 (90/10)**
Speed (rpm)	900	3500
CR	10	20
AFR	50	λ = 2
IMEP (bar)	3.10	8.43
I_{eff} (%)	40.1	42.9
ISFC (g/kW-h)	199.7	149.8
P_{max} (bar)	41.2	143.1
T_{max} (K)	1680	2831
CA50 (deg)	-0.6	0.5
NOx (ppm)	--	1045
HC (g/kW-h)	1.48 e-9	0
CO_2 (g/kW-h)	849.7	0
CO (g/kW-h)	3.75 e-4	0

4.2 Remarks on strengths and limitations of GT-Power for chemical reaction kinetic modeling of HCCI

Despite the complexity of low temperature combustion engines such as HCCI, GT-Power provides a user-friendly interface with the availability of the template model, to facilitate detailed thermodynamic modeling capabilities and execution of HCCI simulations, with detailed combustion process analysis even without user's extensive background in computational fluid dynamics (CFD). Being able to study the transient behaviors of engines, especially how engines responds to varying operating conditions against real time performance and emissions predictions makes this software a highly valuable tool for comprehensive powertrain simulations. Ignition timing control is very important in HCCI engines, likewise achieving accurate predictions are challenging. GT-power might have limitations in accurately capturing ignition timing for HCCI engine models. GT-power 0D model disregards in-cylinder thermal stratification – which has been proven necessary to correctly represent HCCI heat release. In real world conditions, model in GT-power may not account fully for these variations non-homogeneity and spatial variations. Additionally, complex and extensive calibration of HCCI engine parameters (such as fuel injection timing, temperature, CR and ER), may limit achieving accurate simulations and as such, experimental calibration could be done to validate the simulation of HCCI in GT-Power. Feasibility of this current study simulations was validated by benchmarking the results against the base-line HCCI engine fed with n-heptane (diesel surrogate). The result proved that the solver provides stable simulations, for all considered fuel blends and their chemical kinetic mechanisms. Simulation times with multi component mechanism of NH_3, H_2 and n-heptane are on average 32 seconds per cycle with the solver reaching convergence after 6 cycles.

Resulting in-cylinder temperature and pressure of 2831K and 143bar, were relatively high for a HCCI engine and caused increase in engine noise level [27]. Fridhi et al. 2016, studies investigated the effect of intake in inlet air temperate and pressure on the in-cylinder temperature and pressure [28]. They identified that increase in inlet air temperature and pressure reduce the in-cylinder temperature and pressure as well. This could also be studied for further optimization of this NH_3/H_2 fueled HCCI engine. More accurate-absolute level concluding on the combustion phenomenology is reserved for higher-fidelity methods like the UVATZ multizone-model developed by Kakoee et al. [20] to supplement on the drawbacks of single-zone kinetic solver offered by GT-Suite. Overall NOx level was also significantly low, and carbon emission was zero as NH_3/H_2 fuel blend HCCI engines offer new pathways to zero carbon emission.

5. Conclusions

General conclusion regarding the feasibility of GT-suite to investigate the effect of BR, air to fuel ER, and CR on the performance, emission and combustion characteristics of an NH_3/H_2 fueled HCCI engine is presented. The study allowed to draw the following conclusions:

- As little as 10 w/w% of H_2 in the fuel blend could improve the autoignition properties of NH_3.
- Blending H_2 with NH_3, allowed for an increase in engine speed up to about four times the speed of the n-heptane (diesel surrogate) fuel.
- High CR caused excessively high in-cylinder pressure, which might be detrimental to the engine overall efficiency over time.
- With blending ratio of 10%/90% of H_2 /NH_3, a lambda as high as 3 can be achieved without significant penalty on I_{eff}.
- Combustion of NH_3/H_2 blend in excessive air (lean mixture), might present an optimal engine performance and overall efficiency but caused a trade-off effect as engine NOx emissions increased.
- In comparison, the NH_3/H_2 fueled engine offered a better engine performance, overall efficiency and emission characteristics than the n-heptane fueled engine model.
- Results from this study proved that GT-suite chemical kinetic solver provides stable simulations, for all considered fuel blends and their chemical kinetic mechanisms

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DECLARATION OF INTEREST

The author reports financial support was provided by University of Vaasa. The author reports a relationship with University of Vaasa that includes: employment. The author declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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