E3S Web of Conferences **712**, 03002 (2026) https://doi.org/10.1051/e3sconf/202671203002
ICFEE 2026

Methodological Guidelines and Experimental Validation of a Zero-Dimensional Hydrogen Combustion Model in Spark-Ignition Engines.

Pitinan Phuatawee[1,2], *Amnart* Suksri[3,4], *Kritsakon* Pongraktham[2,3], and *Tanakorn* Wongwuttanasatian[1,2,3]*

[1]Energy Engineering Program, Faculty of Engineering, Khon Kaen University, Thailand
[2]Department of Mechanical Engineering, Faculty of Engineering, Khon Kaen University, Khon Kaen, 40002, Thailand
[3]Centre for Alternative Energy Research and Development, Khon Kaen University, Khon Kaen, 40002, Thailand
[4]Department of Electrical Engineering, Faculty of Engineering, Khon Kaen University, Khon Kaen 40002, Thailand

Abstract. This study develops a calibration and validation approach for a zero-dimensional (0-D) combustion model in spark-ignition engines using ANSYS CHEMKIN-Pro 2025R1. The model simulates hydrogen-fueled engine performance under realistic operating conditions, providing a computationally efficient alternative to three-dimensional computational fluid dynamics (CFD) simulations. The model employs the Wiebe function for describing combustion rates and the Woschni correlation for handling heat transfer. A novel Equivalent Overall Heat Transfer (EOHT) concept is introduced to account for combined heat losses through convection, radiation, and cooling systems. Using experimental data from Santiago Molina as a reference, the model was calibrated across excess air ratios (λ) from 1.6 to 2.8. The optimized model demonstrated strong agreement with the experiments for in-cylinder pressure, heat release rate, NOx emissions, IMEP, and combustion duration. Results demonstrate that this 0-D model achieves CFD-comparable accuracy for future hydrogen-ammonia blended fuel combustion modeling with substantially reduced computational costs.

Keyword: Hydrogen, Spark Ignition Engine, Zero Dimensional, CHEMKIN, Calibration, Validation, Energy, Woschni Correlation, Wiebe function

1 Introduction

The global transition from fossil fuels to clean and sustainable energy alternatives has emerged as a critical imperative, particularly within the transportation sector, where internal combustion engines

---

* Corresponding author: tanwon@kku.ac.th

(ICE) remain heavily relied upon across many regions [1, 2]. This issue directly correlates with reducing greenhouse gas emissions and air pollutants such as nitrogen oxides (NOx), which continue to present significant engineering challenges. Among carbon-neutral fuel options, ammonia (NH_3) has garnered increasing attention due to its potential for renewable production, carbon-free molecular structure that eliminates carbon dioxide (CO_2) emissions during combustion, and favorable storage and transport characteristics. NH_3 can be liquefied at −33°C under atmospheric pressure or at room temperature under approximately 0.8–1.0 MPa, making it a practicable hydrogen (H_2) energy carrier compared to direct H_2 storage [3]. However, utilizing NH_3 alone in combustion engines presents substantial limitations, including low ignitability, slow flame propagation rates, and a narrow flammability range [4]. These constraints manifest in actual combustion dynamics through requirements for greater spark advance, delayed peak heat release rates (HRR), and extended combustion durations compared to more reactive fuels. Furthermore, fundamental flame data clearly demonstrate that increasing NH_3 content significantly reduces laminar flame speed [4, 5].

One approach that has been validated both mechanistically and experimentally involves blending H_2 at appropriate ratios with NH_3 to enhance ignitability and accelerate flame propagation without introducing external carbon [5]. Evidence from modeling studies and reaction sensitivity analysis reveals that increasing H_2 content systematically shortens ignition delay time (IDT) and combustion duration, while peaks in-cylinder pressure and HRR shift in directions reflecting more responsive combustion [5]. Nevertheless, utilizing high H_2 fractions encounters practical constraints related to safety, infrastructure, and cost, leading to a trend toward using limited H_2 quantities to promote NH_3 combustion [6].

Methodologically, current research encompasses bench testing, one-dimensional/virtual engine simulations, three-dimensional (3-D) computational fluid dynamics (CFD), and zero-dimensional (0-D) modeling to investigate critical parameters such as IDT and flame speed, subsequently informing design decisions [5,7]. Virtual engine and CFD studies have demonstrated important insights regarding the coupling of chemical mechanisms with semi-empirical correlations to predict NH_3/H_2 fuel combustion performance under realistic engine conditions, while simultaneously employing CFD to understand detailed convective heat transfer and localized turbulence-flame interactions. Additionally, research conducted by Chandrakar et al. (2024) provides a detailed analysis of in-cylinder flow evolution in small spark-ignition (SI) engines (110 cm^3) throughout the intake-compression cycle, correlating findings with fuel-air mixing and combustion through 3-D simulation methods [8]. However, CFD involves substantial computational costs, whereas 0-D/multi-zonal models enable faster parametric testing and exploration of operating condition space, despite offering lower spatial resolution [7]. A study conducted by Ye et al. (2021) focused on the development and testing of 3-D simulation methods for multi-regime combustion in large two-stroke marine dual-fuel engines (natural gas-diesel) with pre-chambers. This research introduces a "mapping method" that connects well-stirred reactors (WSR) with G-equations to achieve both accuracy and computational efficiency [9]. For SI engine applications, the "SI Engine Zonal Simulator" in ANSYS CHEMKIN-Pro has been widely adopted, defining a closed system from intake valve closing (IVC) to exhaust valve open (EVO) and supporting systematic parametric and mechanistic analysis for calibration and validation against experimental data before transferring operating points to detailed CFD analysis.

Based on the above considerations, this research aims to develop a calibration-validation methodology for SI internal combustion engines using 0-D/multi-zonal modeling in ANSYS CHEMKIN-Pro. Although the ultimate objective involves H_2+NH_3 blended fuels, the current configuration of the SI Engine Zonal simulator in CHEMKIN requires complete inputs for the closed system from IVC to EVO (pressure-crank angle/HRR-crank angle profiles, engine geometry, and valve timing). Among the available datasets, only pure H_2 combustion data provide sufficiently comprehensive experimental information [10]. Accordingly, this work focuses on pure H_2 combustion as the foundational step for model calibration and validation before extension toward H_2+NH_3 blended-fuel applications. The goal is to achieve preliminary Woschni heat-transfer correlation coefficients that improve the accuracy of the SI-engine zonal simulation. The results obtained are engineering-comparable to CFD simulations under realistic engine conditions. This approach will reduce simulation time and provide an alternative to 3-D simulations during the preliminary design stage.

2 Methodology

2.1 Model Setup and Reference Benchmarking

This research focused on developing a 0-D model that offers the advantages of rapid combustion simulation using ANSYS CHEMKIN-Pro 2025R1 software. The modeling approach employs the SI Engine Zonal simulator, which provides a 0-D representation as a closed system considered from IVC to EVO, specifically designed to simulate SI internal combustion engines [11]. This study aims to develop a calibration-validation methodology for 0-D modeling to achieve comparable engineering results with 3-D simulations while maintaining computational efficiency. The experimental data reported by Molina et al. (2023), which investigated SI internal combustion engines fueled by H_2 under light-duty conditions [10], were used as the reference benchmark for simulation and calibration. The specifications of the test engine used for model development and parameter tuning are summarized in Table 1.

Table 1. Engine specifications [10].

Parameter	Specifications
Number of cylinders	1
Number of strokes	4
Displaced volume	454.2 cm^3
Stroke	86 mm
Injection systems	PFI/DI
Ignition system	Spark plug
Cylinder diameter	82.0 mm
Compression ratio	10.7
Connecting rod length	144.0 mm
Valves per cylinder	2 intake, 2 exhaust
Engine management system	AVL PREMS GDI
Combustion system	4-valve pent-roof GDI
Intake valve opening (IVO)*	-380 CAD
Intake valve closing (IVC)*	-135 CAD
Exhaust valve opening (EVO)*	-600 CAD
Exhaust valve closing (EVC)*	-338 CAD

Note: *Angles referenced to firing top dead center (TDC) (0 CAD).

The fundamental data required for the simulation includes cylinder geometry, IVC, and EVO timing. Additionally, essential thermodynamic parameters must be specified, such as temperature and pressure at the IVC. These can be calculated retrospectively using Equation 1, where P_{IVC} is the pressure at intake valve closing, P_{TDC} is the pressure at top dead center, CR is the compression ratio, and k is the specific heat ratio of H_2. A temperature-dependent value for H_2 is employed with a specific heat ratio of 1.38 [12].

$$P_{IVC} = \frac{P_{TDC}}{CR^k} \quad (1)$$

For modeling fuel combustion profiles and heat loss characteristics, this study employs widely recognized correlations that are also natively supported within the software. The Wiebe function, which relates to the start of combustion (SOC), burn duration (BD), and Wiebe parameters n and b, is utilized according to Equation 2. For heat loss modeling, the Woschni correlation is applied as shown in Equations 3 and 4, offering high flexibility through adjustable parameters for different cycle phases. A study conducted by Şanlı et al. (2009) showed that the best agreement was achieved using the Woschni correlation, highlighting its significance in model comparisons. The results indicate that the original coefficients (C_1, C_2, and m) can be applied without significant modifications. This formula also accounts for both convective heat transfer and radiation effects in lumped form [13]. The initial parameter values employed in the calculations are listed in Table 2.

$$x_b = f_{combust}(1 - e^{-b\left(\frac{\theta-\theta_0}{\delta\theta}\right)^{n+1}}) \quad (2)$$

$$h = a\ x\ P^b\ x\ w^b\ x\ \ B^b\ x\ T^c \quad (3)$$

$$w = \left(\left(C_{11} + \frac{C_{12}v_{swirl}}{S_p}\right)\right)S_p + C_2(\frac{v_d T_i}{P_i V_i})(P - P_{motored}) \quad (4)$$

Table 2. Initial parameter values used for calibration

Parameter	Initial value
Wiebe function b	5 (default)[c]
Wiebe function n	2 (default)[c]
Coefficient a	3.26/Bore [m][a]
Coefficient b	0.8 (Woschni requirement) [b]
Coefficient c	-0.53 (Woschni requirement) [b]
Coefficient C_{11} (Compression interval)	2.28[b]
Coefficient C_{11} (Combustion interval)	2.28[b]
Coefficient C_2 (Combustion interval)	0.324 cm/sec K [b]
Coefficient C_{11} (Expansion interval)	2.28[b]
Coefficient C_2 (Expansion interval)	0.324 cm/sec K [b]

Note: [a]Since the typical recommended value of a is 3.26, but the software uses a different formulation: $a_{equivalent}$ = 3.26/Bore[m]
[b]Referenced from [13]
[c]Referenced from [11, 15]

Preliminary simulations using default Woschni parameters revealed that the heat loss calculated by the Woschni correlation was minimal, accounting for only 0.0057% of fuel heat release. This value is significantly lower than findings reported in the literature, which indicate that heat transfer to cylinder walls in spark-ignition engines, including the expansion phase over the entire cycle, typically represents 10-15% of fuel energy [14], as illustrated in Figure 1.

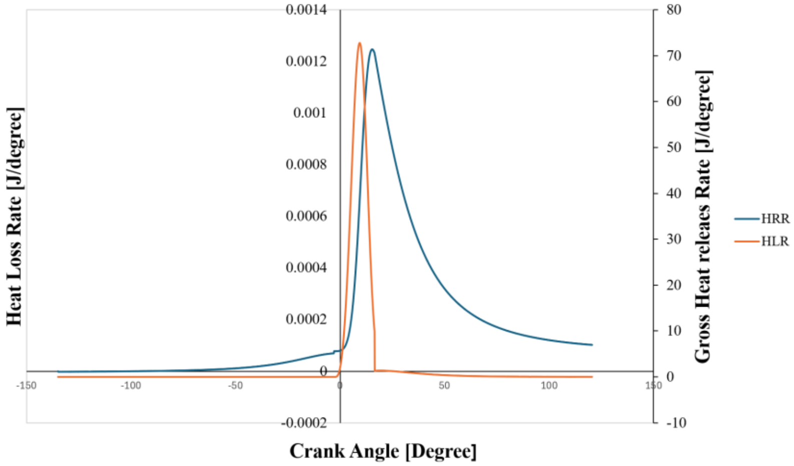

Fig.1. Comparison of the heat loss rate (HLR) and HRR

Based on the above findings, it is necessary to calibrate the heat transfer correlation and validate the results against actual experimental data from Molina's research [10]. This study proposes an approach for adjusting Woschni correlation parameters beyond the original consideration of only convective and radiative heat transfer, which proved insufficient for capturing total heat loss in the simulations. Instead, a new concept termed Equivalent Overall Heat Transfer (EOHT) is introduced, consolidating heat losses from convection, radiation, cooling water dissipation, and other sources into a unified parameter for simulation in the CHEMKIN 2025R1 SI Engine Zonal model. A validated reduced reaction mechanism is employed [15].

2.2 Procedure for Model Calibration and Validation

The calibration process begins by adjusting the mass burned fraction (MBF) to match the experimental data [10] using the Wiebe function described in Equation 2. Parameters n and b are utilized to modify the shape of the combustion profile, which includes CA10, CA50, and CA90. The initial values are set according to the recommendations in the CHEMKIN manual, specifically at 2 and 5, respectively. Once the combustion profile has been calibrated, the pressure-crank angle profile must be verified for agreement with experimental data. If deviations remain, the HLR is examined relative to the gross heat release rate (GHRR) until the ratio is lower than 10%. The Woschni correlation parameters are then recalibrated using the initial values from Table 3 to better align the HRR profile with experimental observations. After completing the calibration of both the combustion and heat-transfer submodels, the validation analysis is performed using additional datasets at different excess air ratios ($\lambda = 1.6, 2.0, 2.4$, and 2.8). The model performance is assessed based on pressure–crank-angle and heat-release profiles, indicated mean effective pressure (IMEP), NOx trends, peak HRR, and MBF. The overall calibration–validation procedure is summarized in the workflow diagram, as shown in Figure 2.

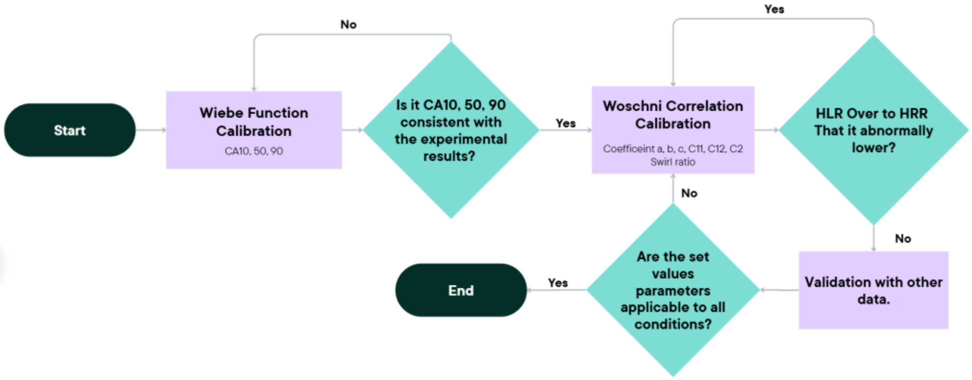

Fig.2. Workflow diagram

3 Results and Discussion

3.1 Model calibration results

This section presents the calibration results of the Wiebe and Woschni correlations to optimize combustion and heat transfer characteristics. The calibration results between before and after for the Woschni correlation in wall heat transfer are shown in Table 3. As mentioned in section 2.2, the initial values following Woschni's recommendations before adjustment yielded a significantly lower HLR relative to the HRR. After calibrating both the Woschni correlation parameters and the MFB profile, optimized values were obtained under conditions of $\lambda = 1.6$ with 99.99% H_2 fuel. These values result in a pressure-crank angle and HRR profiles closely aligned with the literature, as displayed in Figure 3.

Table 3: Parameter values before and after calibration

Elements	**Parameter Woschni Correlation Requirement**	**Parameter Woschni Correlation After Calibration**
Dimensional Heat Transfer Correlation $h = a\ x\ P^b\ x\ w^b\ x\ B^b\ x\ T^c$		
Coefficient a	3.26/Bore [m]	3.26/Bore [m]
Coefficient b	0.8	0.8
Coefficient c	-0.53	-0.26
Woschni Correlation Parameter		
Compression coefficient C11	2.28	228
Compression coefficient C12	0	0
Compression coefficient C2	0	0
Ratio of swirl velocity to mean piston speed	0	0
Combustion coefficient C11	2.28	228
Combustion coefficient C12	1.15	115
Combustion coefficient C2	0.324 [cm/sec K]	32.4 [cm/sec K]
Ratio of swirl velocity to mean piston speed	0.5	50
Expansion coefficient C11	2.28	228
Expansion coefficient C12	1.2	120
Expansion coefficient C2	0.324	32.4
Ratio of swirl velocity to mean piston speed	0.5	50

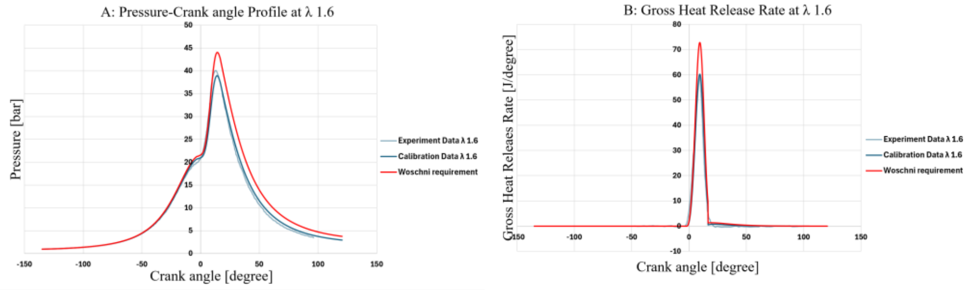

Fig.3. The calibration results between the data from experimental data [10], recommended Woschni correlation values [13], and calibrated Woschni correlation, (A) pressure-crank angle profile, and (B) HRR profile.

3.2 Model Validation and Performance Assessment

The calibrated model was validated using experimental datasets by Molina et al. (2023) [10] at excess air ratios of λ = 1.6, 2.0, 2.4, and 2.8. Validation metrics included pressure-crank angle profiles, HRR profiles, IMEP, NOx trends, maximum HRR, and MFB. Statistical comparison using the determination coefficient (R^2) and normalized root-mean-square error (nRMSE) confirmed strong agreement between simulation and experiment, as shown in Figure 4. The pressure-crank angle correlations for λ values of 1.6, 2.0, 2.4, and 2.8 achieved R^2 values of 0.9920, 0.9956, 0.9982, and 0.9979, with nRMSE values of 0.0272, 0.0328, 0.0396, and 0.0451, respectively. These metrics indicate minimal deviation and excellent agreement.

In the validation of MFB, burn duration, IMEP, and maximum HRR, Two One-Sided Tests (TOST) with 90% confidence intervals were employed. Equivalence margins of ±1 Crank Angle Degree (CAD) for CA10/50/90, ±2 CAD for burn duration, ±0.15 bar for IMEP, and ±2 J/deg for maximum HRR were established as sufficiently narrow thresholds. TOST analysis confirmed that all parameters passed equivalence testing within these margins, as illustrated in Figure 5.

Finally, the NOx validation utilized absolute error (AE) as a metric. Results showed a progressively decreasing error with increasing the excess air ratio, achieving the closest agreement at λ = 2.8 with AE = 0.284 g/kWh, as presented in Figure 6. This demonstrated a consistent trend in improving accuracy with leaner emissions.

In summary, the developed 0-D combustion model shows good agreement with experimental data and 3-D CFD results ($R^2 > 0.99$). It also requires far less computation time, generally running hundreds to thousands of times faster than detailed 3-D simulations, which makes it suitable for preliminary design studies and parametric analyses of λ, spark timing, and EGR. Although the 0-D approach cannot capture spatial details or localized phenomena, the calibrated parameters provide sufficiently reliable initial settings for subsequent CHEMKIN simultions.

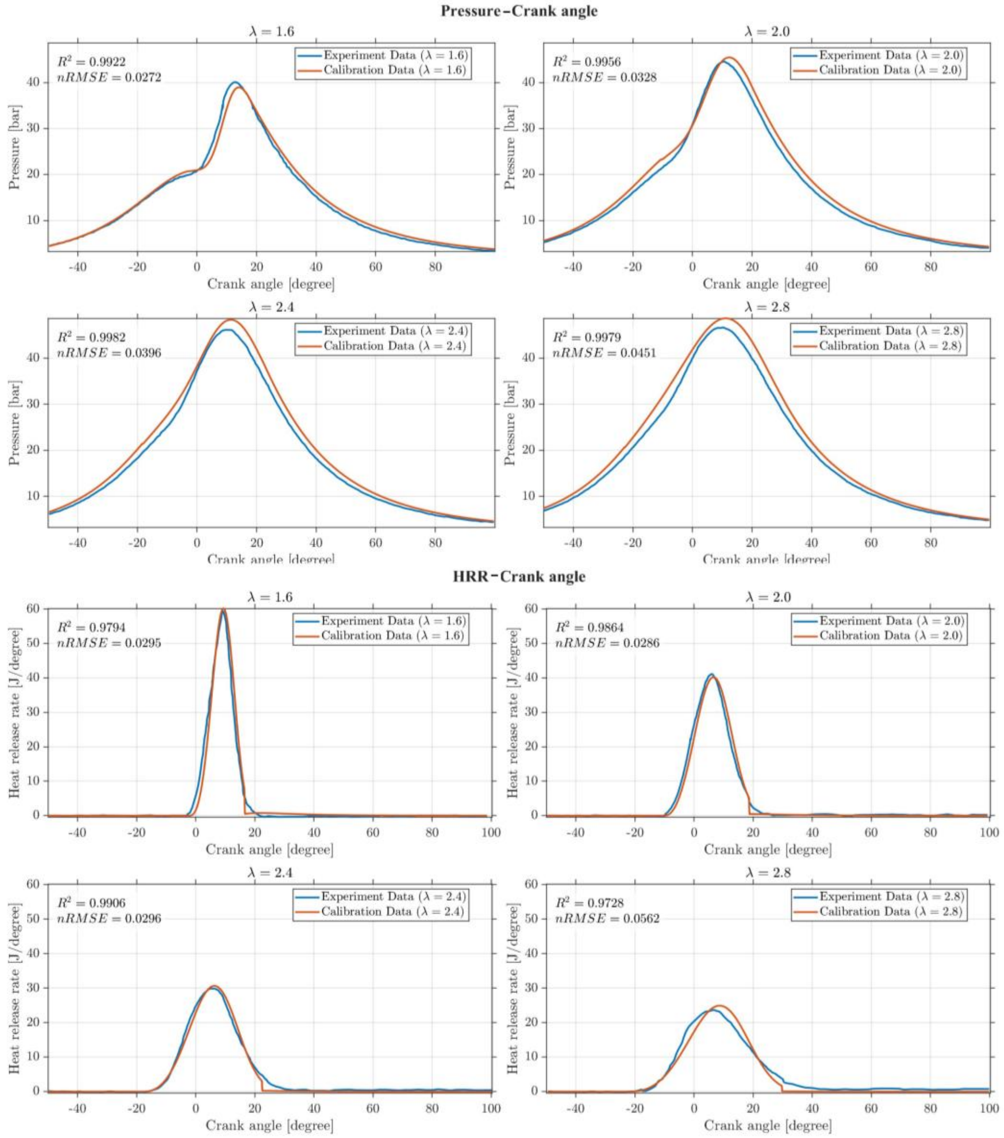

Fig.4. Pressure-Crank Angle profiles and HRR at different excess air ratios of λ = 1.6, 2.0, 2.4, and 2.8

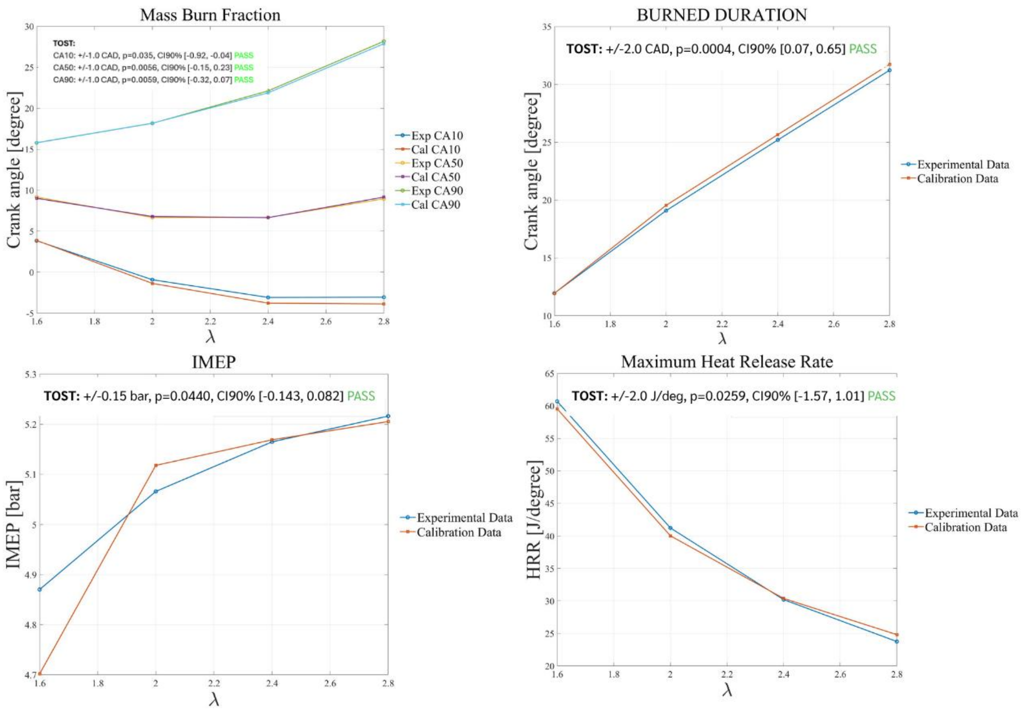

Fig.5. Comparison and validation considering MFB, burn duration, IMEP, and maximum HRR at excess air ratios of λ = 1.6, 2.0, 2.4, and 2.8

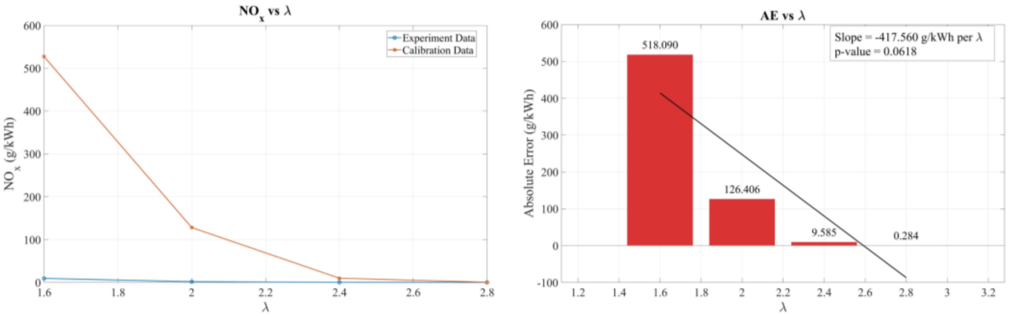

Fig.6. NOx–λ validation, (a) experiment vs calibrated model, and (b) AE vs λ with linear fit. Error decreases at leaner mixtures (slope ≈ −417.56 g/kWh per λ; AE at λ=2.8 = 0.284 g/kWh).

4 Conclusion

This study developed and validated a 0-D multi-zonal combustion model for an H_2-fuelled SI engine using ANSYS CHEMKIN-Pro 2025R1. A systematic calibration–validation procedure was established by integrating a Wiebe-based MBF formulation with an extended Woschni heat-transfer correlation. The calibrated model successfully simulated in-cylinder pressure tracing, HRR, and combustion phasing using experimental data from the reference engine operating under lean conditions (λ = 1.6–2.8), showing a strong correlation with IMEP and trends in NOx emissions. Additionally, the optimized correlation corrected the heat loss under-prediction observed with default Woschni parameters.

Compared with a full 3-D CFD, the proposed 0-D approach cannot resolve complex problems, such as spatial inhomogeneities, local flow structures, or detailed turbulence–chemistry interactions. Once properly calibrated, it delivers global performance indicators comparable to CFD, including pressure traces, heat release behavior, combustion phasing, IMEP, and NOx emissions, at lower computational resources. This makes the 0-D model particularly valuable as a rapid screening and design tool for parametric studies involving excess air ratio, spark timing, and exhaust gas recirculation (EGR) during the preliminary design stages, before committing to computationally expensive 3-D CFD simulations for a limited set of representative cases.

The present work was conducted for a specific engine geometry operating at 1500 rpm with high-purity hydrogen fuel. As a result, the optimized coefficients should be considered as a physics-based baseline rather than universal constants. According to the results, the methodology and the calibrated parameter set provide a practical foundation for future extensions toward H_2–NH_3 blended fuels and advanced combustion strategies, such as pre-chamber ignition. Future studies should apply the established calibration–validation framework in H_2–NH_3 mixtures to identify optimal H_2 support ratios, λ values, and EGR levels that enable stable ultra-lean combustion while minimizing NOx emissions and controlling NH_3 slip. This comprehensive understanding will significantly contribute to the advancement of carbon-neutral H_2–NH_3 fueled SI engines, which promote environmentally friendly and sustainable advanced combustion technologies.

Supported by Research Program funding, from Research and Innovation Department Khon Kaen University. The research team would like to thank the Center of Alternative Energy Research and Development, Khon Kaen University, for supporting our work.

References

1. N. Abu-Hamdeh, K. Alnefaie, K. Almitani, Appl. Sci. **9**, 4597 (2019)
2. N. Abu-Hamdeh, K. Alnefaie, K. Almitani, Appl. Sci. **7**, 1001 (2017)
3. A.J. Reiter, S.C. Kong, ACS Sustainable Chem. Eng. **5**, 9784 (2017)
4. C. Tao, Z. Dan liang, AIAA J. **61**, 7 (2023)
5. H. Guo, W. Liu, Y. Yu, et al., Int. J. Hydrogen Energy (2023)
6. R. Zhang, A. Hayakawa, Appl. Therm. Eng. (2023)
7. F. Berni, V. Pessina, L. Teodosio, A. d'Adamo, M. Borghi, S. Fontanesi, Int. J. Hydrogen Energy **50**, 908 (2023)
8. C.K. Chandrakar, K. Ayyanar, V.S., T. Anand, M. Mittal, J. Eng. Gas Turbines Power **146**, 10 (2024)
9. Y. Ye, Z. Yue, H. Wang, H. Liu, C. Wu, M. Yao, Energies **14**, 6126 (2021)
10. S. Molina, R. Novella, J. Gomez-Soriano, M. Olcina-Girona, Appl. Sci. **13**, 12055 (2023)
11. Q.N. Minh, Ansys Chemkin Tutorials 2024 R1 (Scribd, 2024
12. O.A. Marzouk, Int. J. Aeronaut. Sci. Aerosp. Res., 150 (2018)
13. A. Sanli, C. Sayin, M. Gumus, I. Kilicaslan, M. Canakci, Numer. Heat Transfer, Part A **56**, 444 (2009)
14. H. Pernet, Internal-Combustion Engine Heat Transfer (Flèches, 2015)
15. G. Grassi, L. Vervisch, P. Domingo, Combust. Flame **279**, 114287 (2025)