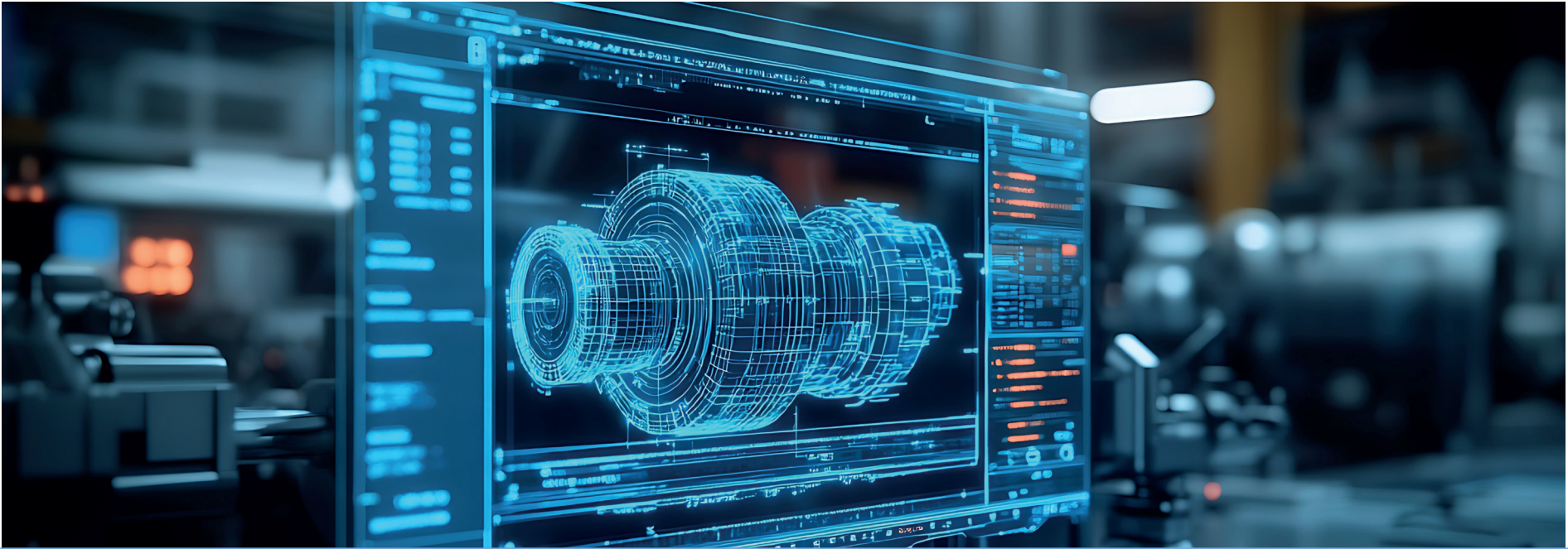




AI-ASSISTED MODELING, DESIGN OPTIMIZATION, AND KNOCK DETECTION FOR ALTERNATIVE-FUELED INTERNAL COMBUSTION ENGINES

The objective of this review is to investigate recent studies applying artificial intelligence for modeling, design optimization, calibration, and knock detection of ICEs using alternative fuels such as hydrogen, ammonia, ethanol, biodiesel, and CNG. The abilities of genetic algorithms, statistical optimization tools, and machine learning models such as artificial neural networks, random forests, and convolutional neural networks are examined in this review. Studies were identified by searching keywords related to alternative fuels, engine development, and AI on academic search engines and databases including Google Scholar and ScienceDirect. Included studies must have been published between 2022 and 2026 and must apply one or more intelligent algorithm(s) to a facet of engine development. Across the selected studies, machine-learning models reduced computation time or supported multi-objective optimization under defined datasets and operating conditions, but their accuracy and generalizability remained dependent on the training domain, inputs, validation method, and implementation. Some alternative fuels can be prone to engine knock, which deep learning models like CNNs have been able to classify with a 74.5% overall accuracy. This review will discuss and analyze the results of each study, after which a limitations section and concluding thoughts will be provided. In summary, the studies are limited by lack of independent validation and the results of each study are constrained to the specific operating conditions and fuel type(s) tested.

Introduction

For decades, internal combustion engines have been integral to the global transportation sector. As resources continue to dwindle, there is a growing sentiment to cut reliance on fossil fuels and shift toward alternative sources of energy for engines [1]. Despite their benefits, many popular alternative fuels negatively impact engine performance or require internal modifications to properly implement. This review focuses on a select few of these fuels, namely hydrogen, ethanol, ammonia, biodiesel, and compressed natural gas. Hydrogen is prone to abnormal combustion phenomena, while ethanol requires high in-cylinder temperatures for ignition [2, 3]. Biofuels suffer from poor engine efficiency and can increase NOx emissions [4]. Maximizing the utility of these fuels requires in-depth investigations that AI can facilitate. In this paper, AI refers to computational systems capable of managing complex relationships and identifying optimal solutions. These include predictive ML models as well as optimization tools. The studies discussed in this review illustrate AI's suitability for the modeling, design, calibration, and knock detection of ICEs.

Modeling and Simulation

Many alternative fuels have displayed benefits for engine efficiency and overall sustainability. For these reasons, hydrogen continues to gain popularity as an alternative fuel source. However, its low H2 density, high flame temperatures, and

propensity for knock create problems that require strict control over the combustion process [5]. Accurate predictions of in-cylinder pressure and combustion speed can aid in preventing issues such as backfire, misfires, delayed combustion, knocking, and increased NOx emissions [6, 7]. Ricci et al. (2025) tested the in-cylinder pressure prediction capability of an ANN against that of GT-POWER, a traditional simulation tool used for the same task. For this study, GT-POWER required detailed specifications of engine parameters, which proved to be both time and resource intensive. This is noted to limit its viability for real-time applications. In comparison, a BPANN was deployed for the same task, using layers to receive, process, and make predictions based on three distinct datasets including injection/ignition timing, air-fuel ratio, and torque. The BPANN used a feed-forward architecture with error backpropagation during training, as shown in Figure 1. As such, the model does not outright eliminate the need for optical measurements but may reduce the need for repeated camera testing. Using an RMSE metric as a comparison tool, the authors found that the BPANN demonstrated error percentages of less than half those of GT-POWER; however, this was true in only two of the three tested cases. Nonetheless, the authors conclude that integrating machine learning approaches in combustion systems can enhance both the accuracy and efficiency of prediction tasks [6].

A 2024 paper by Banta et al. applied and compared various ML models for computing the turbulent combustion speeds of hydrogen-natural gas engines. The models tested included an MLR, SVR, RF, and ANN model. The models used measurable engine parameters, including dimensionless flame radius, H2 percentage, air-fuel ratio, and engine speed, as inputs. When evaluating the model outputs against experimental data, the RF and ANN models were found to have the highest accuracy based on RMSE. Additionally, all models obtained significantly lower calculation times than GRI-Mech 3.0, an established combustion modeling mechanism used in the study for comparison purposes. Despite this improvement in computation speed, the models are less robust than GRI-Mech 3.0, which limits their versatility across different fuel types. This also means that these results are specifically tied to the operating conditions and fuel type tested in the study [7].

It is worth noting that in-cylinder pressure can depend on the speed at which combustion occurs, meaning combustion speed can indirectly alter BMEP, a core component of engine performance. Based on the studies from Ricci et al. and Banta et al., an RF model can be employed for real-time combustion speed estimation while an ANN model estimates subsequent in-cylinder pressure [6, 7]. This is a potential approach that may be beneficial to consider for future research.

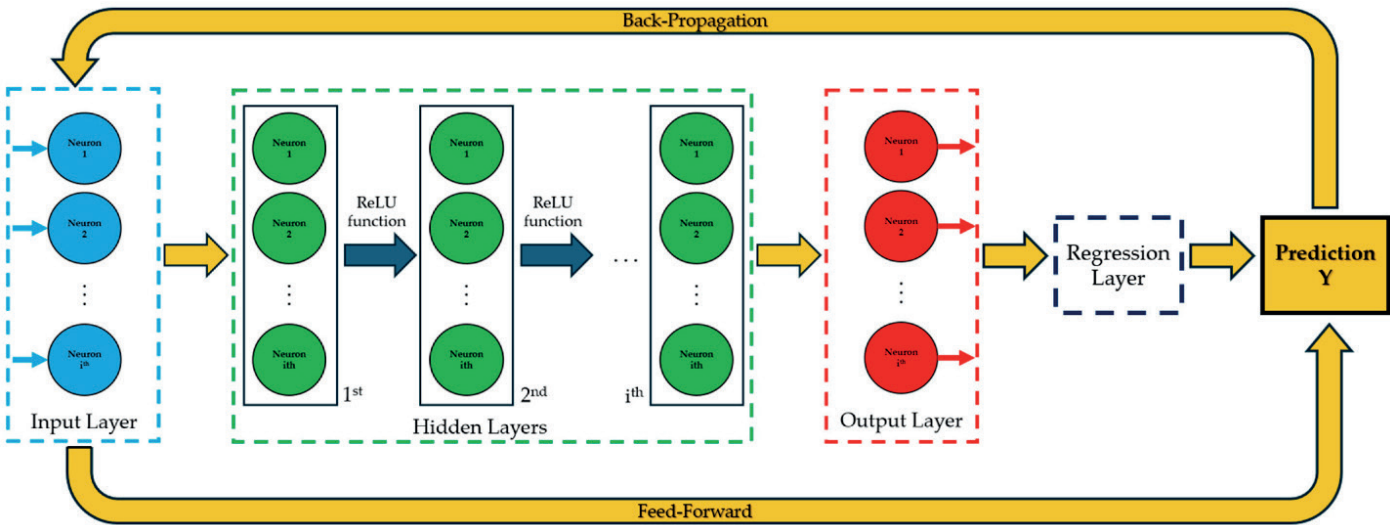


Figure 1. Conceptual layout of the BPANN
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Acronyms

Acronym	Definition
AI	Artificial intelligence
ANN	Artificial neural network
BMEP	Brake mean effective pressure
BOpt	Bayesian optimization
BPANN	Back-propagation artificial neural network
BSFC	Brake-specific fuel consumption
BTE	Brake thermal efficiency
CA bTDC	Crank angle before top dead center
CI	Compression-ignition
CNG	Compressed natural gas
CNN	Convolutional neural network
CO	Carbon monoxide
CO ₂	Carbon dioxide
CRDI	Common rail direct injection
DoE	Design of experiments
ECU	Electronic control unit
EGR	Exhaust gas recirculation
GA	Genetic algorithm
HC	Hydrocarbons
HCNG	Hydrogen-enriched compressed natural gas
ICE	Internal combustion engine
ICM	Ignition control module
MAPO	Maximum amplitude pressure oscillation
ML	Machine learning
MLR	Multiple linear regression
NH3	Ammonia
NSGA-II / NSGA-III	Non-dominated sorting genetic algorithm II / III
NOx	Nitrogen oxides
PSO	Particle swarm optimization
PSO-SVM	Particle swarm optimization-support vector machine
RF	Random forest
RMSE	Root-mean-square error
RSM	Response surface methodology
SI	Spark-ignition
SVR	Support vector regression
SVM	Support vector machine
TOPSIS	Technique for order preference by similarity to ideal solution
UHC	Unburned hydrocarbons

Design Optimization

One way of improving the performance of alternative fuels involves optimizing the design of engines. For CI engines, this can be done via modifying piston bowl geometry, which can significantly influence combustion quality [8]. These changes can improve thermal efficiency and combustion processes for both alcohol-based and non-alcohol-based fuels [3, 9].

Tekg l et al. (2023) applied BOpt to identify the optimal piston bowl geometry for an ethanol-fueled heavy-duty CI engine. The optimization was done on a dataset of 165 sample designs obtained through DoE. Using a fixed spray injector angle, BOpt identified a design that increased indicated thermal efficiency by 1.90 percentage points relative to the baseline while using 35% fewer evaluated samples than the DoE approach. It is important to note that for this specific study, the low soot properties of the tested alcohol fuel facilitate NOx aftertreatment. As such, the sole criterion selected for optimization in this study was indicated thermal efficiency [3]. Non-alcohol alternative fuels such as ammonia do not have the same properties that facilitate NOx reduction. In such cases, genetic algorithms can be used to weigh different criteria.

Sehili et al. (2024) applied a multi-objective approach to optimize piston bowl shape and swirl rate in an ammonia-diesel engine. The workflow involved generating a set of designs with Latin Hypercube Sampling, after which 3D modeling was used to build the designs and an ANN model was constructed. An ANN meta-model was trained to link performance and emissions with the bowl shape and swirl rate parameters, after which NSGA-II ranked the candidate solutions via non-dominated sorting. Figure 2 illustrates the bowl shape and swirl rate parameters that were modified for each design. The optimal configuration of piston bowl geometry and swirl rate reduced unburned ammonia by over 43%. Relative to the ammonia–diesel base case, Case 1, targeting efficiency optimization, increased indicated thermal efficiency from 29.8% to 38.7%—approximately 30%—and increased NO_x from 4.85 to 8.34 g/kWh—approximately 72%. A second design optimizing

emissions, Case 2, successfully reduced NOx emissions from both the base case as well as Case 1. Table 1 illustrates the changes in parameters P, b, d, and S, shown in Figure 2, and corresponding indicated thermal efficiency, η_{th} , as well as combustion efficiency, eff_{comb} . The authors also enriched the fuel in Case 2 with hydrogen, achieving an improvement in thermal efficiency of 32% from the base case with a 26% increase in NOx. Due to the nonlinear relationships between piston bowl parameters and engine performance, it is favorable to use multivariable optimization to identify optimal parameters. AI is useful for this task due to its ability to handle conflicting objectives [9].

Figure 2. (a) bowl deformation range and (b) deformation control parameters
Reproduced from [9], licensed under CC BY 4.0

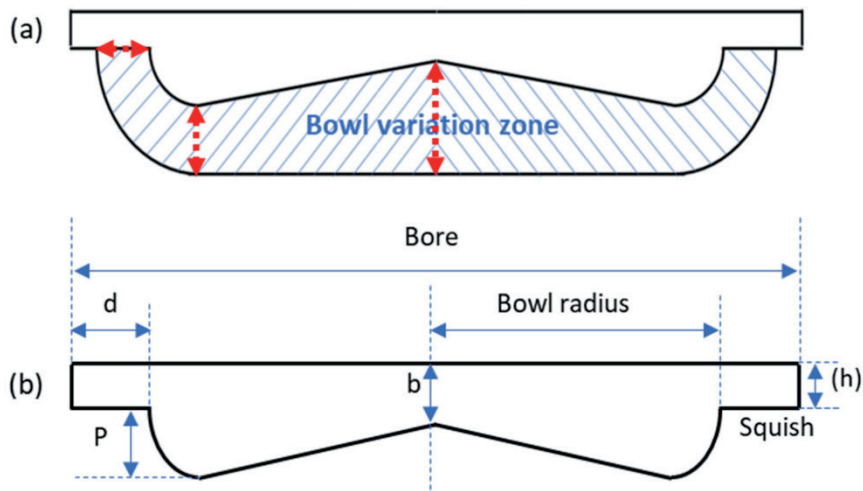


Table 1. Comparison of piston bowl parameters and outputs between reference operation cases

Case	P	b	d	S	NOx (g/kWh)	η_{th} (%)	eff_{comb} (%)
NG/D case	–	–	–	4.5	7.92	34.8	93.4
Base case	–	–	–	4.5	4.85	29.8	67.3
Case 1	9.857	11.208	3.319	7.842	8.34	38.7	95.8
Case 2	8.466	8.317	6.758	2.951	3.08	30.6	65.3

Adapted from [9]

Testing and Calibration

Engine calibration involves optimizing fuel efficiency and minimizing pollutant emissions to achieve peak engine performance [10]. AI-based strategies have been useful for calibration tasks involving emissions reduction and combustion optimization [11].

In recent years, ethanol has gained increased attention as an alternative fuel for its highly renewable nature. To maximize its performance in engines, researchers use AI-based approaches to optimize and calibrate engine control parameters. Zhu et al. (2025) trained an RF model to predict torque and emission levels from seven input parameters in an ethanol-water-fueled engine. Using NSGA-II, Pareto fronts were found between pairings of torque and CO, CO₂, HC, and NOx emissions. A five-objective optimization, performed using NSGA-III, also revealed the best compromise considering all five variables. Table 2 provides a summary of the Pareto fronts identified between different variable combinations. The authors note that their two-phase approach enables efficient optimization when conflicting objectives, such as maximizing torque and minimizing emissions, are present [12].

Table 2. Comparison of Optimization Combinations

Optimization combination	Torque (Nm)	CO (ppm)	CO ₂ (ppm)	HC (ppm)	NOx (ppm)
Torque – CO ₂	12.29	–	8.81	–	–
Torque – CO	12.14	0.39	–	–	–
Torque – HC	12.24	–	–	12.56	–
Torque – NOx	12.11	–	–	–	46.43
Five-objective	11.10	0.36	8.72	65.86	495.66

Compiled from [12]

Biodiesel is another popular renewable fuel which can be improved with the addition of hydrogen. To investigate hydrogen's effects on biodiesel, Goud and Baba (2026) applied a multi-step optimization process to calibrate injection timing and pressure in a hydrogen-enriched biodiesel engine. Similar to Sehili et al., an ANN and NSGA-II combination was used to predict outcomes and optimize configurations based on a dataset of 162 experimental observations from D100, PKME20, and PKME20H10 blends. Afterward, TOPSIS was employed to identify the best compromise between thermal efficiency and emissions for the resulting solutions. The optimal configuration was identified at 25°CA bTDC with 512 bar injection pressure, resulting in notable reductions in CO, UHC, and smoke opacity relative to the diesel baseline. Afterward, experimental testing revealed relatively low error percentages between the experimental values and computational results, highlighting the accuracy of the AI method. The authors also suggest that ANNs may be superior in handling nonlinear variable relationships compared to alternative tools like RSM, GA, and PSO, although this comparison was not directly investigated in the study [4].

Knock Detection and Prediction

Alternative fuels such as hydrogen can be prone to knock, an abnormal combustion phenomenon that occurs when the in-cylinder air-fuel mixture spontaneously ignites [2, 13]. This causes the cylinder to resonate, producing pressure oscillations that result in engine damage and reduced performance [13]. AI methodologies have been used to both identify and predict knock in alternative-fueled engines.

The “gold standard” for combustion diagnostics involves using in-cylinder pressure sensors, which can be constrained by cost. An alternative method involves using ion current measurements for in-cylinder pressure diagnostics. Ion current can be fed into deep learning models, such as CNNs, which then use it to classify knock. A 2024 study by Björnsson and Tunestål employed this strategy to classify knocking combustion in a CNG engine. For its input, the CNN model used ion current, measured with the ICM, to classify knock. It also used the in-cylinder pressure to calculate Maximum Amplitude Pressure Oscillation (MAPO) values that establish the no-knock, medium-knock, and heavy-knock categories. The output of the model corresponded to one of these categories based on the received ion current. In distinguishing between the three knock classes, the model had an overall accuracy of 74.5%. As can be seen in Table 3, the model had success rates of over 60% in determining the correct severity of knock [13].

Table 3. Knock Severity Identification

True Class \ Predicted Class	No-Knock (Predicted)	Medium-Knock (Predicted)	Heavy-Knock (Predicted)
No-Knock (True)	229 (87.40%)	31 (11.83%)	2 (0.76%)
Medium-Knock (True)	42 (16.03%)	177 (67.56%)	43 (16.41%)
Heavy-Knock (True)	3 (1.15%)	76 (29.01%)	183 (69.85%)

Adapted from [13]

Knock prediction using AI has also been investigated alongside alternative-fueled engines. Farhan et al. (2024) trained a PSO-SVM model to predict knock intensity in a CNG engine enriched with hydrogen. The model successfully found the relationships between engine speed, engine load, EGR rate, spark timing, hydrogen amount, and knock intensity. These relationships, among other results, are illustrated in Table 4. It was also observed that using all input parameters resulted in significantly more accurate predictions than using one input, with little effect on computation time. Based on the results, the authors suggest that implementing AI algorithms in vehicle ECUs may be beneficial, given their potential to accurately predict knock. However, this was not directly validated in the study [14].

Table 4. Effect of Input Parameters on Engine Performance and Knock Characteristics

Input Parameter	Range	Output Parameter	% Change
Hydrogen amount	0–40%	In-cylinder pressure	+ 32.7%
Load	25–100%	In-cylinder pressure	+75.8%
Engine speed	1100–1700 rpm	In-cylinder pressure	-12.19%
Hydrogen amount	0–40%	In-cylinder heat transfer rate	+21.5%
Hydrogen amount	0–40%	Knock intensity	+7.6%
Hydrogen amount	0–40%	Knock ratio	+33.5%
Hydrogen amount	0–40%	Exhaust temperature	+6.4%
Load (1200 rpm)	25–100%	In-cylinder heat transfer rate	+77.8%
Load (1200 rpm)	25–100%	Knock intensity	+69.8%
Load (1200 rpm)	25–100%	Knock ratio	+88.2%
Load (1200 rpm)	25–100%	Exhaust temperature	+46.7%
Engine speed	700–1700 rpm	In-cylinder heat transfer rate	-47.2%
Engine speed	700–1700 rpm	Knock intensity	-38.9%
Engine speed	700–1700 rpm	Knock ratio	-36.06%
Engine speed	700–1700 rpm	Exhaust temperature	-14.1%

Compiled from [14]

Limitations

The results of each method are tied to the fuel blend, engine type, and operating conditions of their respective study. As outlined by Banta et al., the success of the ML models investigated in their study cannot be comfortably established for fuel types outside of HCNG engines. Several techniques also continue to rely on optical or sensor-driven data, notably the machine learning models discussed by Ricci et al. and Björnsson and Tunestål. For these reasons, conventional techniques may still be comparable to or favorable over AI-based methods depending on the circumstances. The dataset sizes vary across the studies but typically range in the hundreds in terms of data points or engine cycles. Some methodologies omit specific information about inputs or data sizes, as is the case with Sehili et al., which limits their reproducibility in another study. In terms of model interpretability, the ML models discussed in these studies do not always reveal their internal logic. Notably, Banta et al. state that although their SVR model can be trained accurately, it is an extension of SVM, which does not provide users with a physical understanding of its system. Several other models, including the CNN used by Björnsson and Tunestål and the BPANN discussed in Ricci et al., can be considered black-box models due to their complex and difficult-to-trace layers. Lastly, the studies discussed in this review have not been independently validated, leaving results subject to uncertainty. Similarly, suggestions to implement AI in vehicle ECUs and real-time monitoring systems, like those of Farhan et al., require further investigation to be verified.

Conclusion

As alternative fuels continue to rise in popularity, the issue of optimizing them for practical application becomes increasingly relevant. New research highlights AI’s suitability for this task, albeit with limitations. In the selected studies, some machine-learning models reduced calculation time or supported optimization relative to the specific comparison methods used, although performance remained dependent on the training data, fuel, engine, and implementation. For design and calibration tasks, one strategy shared across various studies involves pairing machine learning models with optimization algorithms, such as ANN with NSGA-II. This approach is especially useful for balancing the performance and emissions between fuels, which often involves identifying a Pareto front between various objectives. AI-based knock classifiers showed promising study-specific performance, but they continued to rely on sensor inputs and require broader validation across fuels, engines, and operating conditions. One direction of future research should be to investigate the RF-ANN hybrid strategy proposed in the review. Additionally, results obtained from the studies discussed should be independently verified across a variety of operating conditions to ensure they hold true for different applications. Lastly, the suggestion to implement AI in vehicle ECUs, as highlighted by Farhan et al., should be investigated to determine AI’s suitability for real-time performance monitoring tasks.

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Table 5a. Comparison of fuels, engines, models, inputs, and outputs

Study	Fuel	Engine	Model(s)	Inputs	Outputs
Ricci et al. (2025)	Hydrogen	Single-cylinder	Back-propagation ANN	Injection/ignition timing, air-fuel ratio, torque	In-cylinder pressure, equivalent flame radius
Banta et al. (2024)	Hydrogen-natural gas blends	Single-cylinder, spark ignition	MLR, SVR, RF, ANN	Dimensionless flame front radius, % H2, fuel-air equivalence ratio, engine speed ANN-specific: turbulence intensity, laminar combustion speed, thermal diffusivity, kinematic viscosity, Prandtl number	Turbulent combustion speed
Tekgül et al. (2023)	Ethanol	Heavy-duty CI engine	Bayesian optimization	Piston bowl geometry, fixed spray injector angle	Indicated thermal efficiency
Sehili et al. (2024)	Ammonia-diesel	Single cylinder, four-stroke, CI engine	ANN + NSGA-II	3D-modeled piston bowl designs (not explicitly stated)	Thermal efficiency, unburned ammonia, NOx
Zhu et al. (2025)	Ethanol-water	Single cylinder Otto cycle engine	RF + NSGA-II/NSGA-III	Water fraction, rotational speed, compression ratio, ignition advance angle, fuel/exhaust/oil temperature	Torque, CO, CO ₂ , HC, NOx
Goud and Baba (2026)	Hydrogen-enriched biodiesel	Single-cylinder CRDI diesel engine	ANN + NSGA-II + TOPSIS	Load, injection pressure/timing, fuel type, hydrogen flow rate	BTE, BSFC, UHC, CO, smoke opacity, NOx
Björnsson and Tunestål (2024)	Compressed natural gas	Heavy-duty spark ignition engine	CNN	Ion-current, in-cylinder pressure trace	Knock classification (no-knock, medium, heavy), MAPO quantity
Farhan et al. (2024)	Hydrogen-enriched compressed natural gas	Six-cylinder engine	PSO-SVM	Engine speed, engine load, EGR rate, spark timing, hydrogen amount	Knock intensity

Compiled from [3], [4], [6], [7], [9], [12], [13], [14]

Table 5b. Comparison of validation results, benefits, and limitations

Study	Validation result	Benefits	Limitations
Ricci et al. (2025)	In-cylinder pressure: ANN RMSE < 0.44%, GT-POWER RMSE 0.92%-1.57% Equivalent flame radius: ANN RMSE <3%	Lower error than GT-POWER in 2/3 cases, reduces camera testing	Still requires optical measurements
Banta et al. (2024)	RMSE values on standardized dataset: 2.5881 for MLR, 2.0715 for SVR, 0.4274 for RF, 0.5918 for ANN. Calculation time <1s for MLR, SVR, RF (~6.42s for ANN), ~39,782s for GRI-Mech 3.0	Faster than GRI-Mech 3.0, accurate results and easy implementation depending on model	Reduced robustness outside of studied fuel type
Tekgül et al. (2023)	Up 1.90 percentage points in indicated thermal efficiency from baseline, 35% fewer samples than DoE	Improved thermal efficiency, fewer data samples than DoE	Does not account for criteria outside of thermal efficiency
Sehili et al. (2024)	Case 1: +30% thermal efficiency relative to base case Case 2 (w/ H2): +32% thermal efficiency Optimal configuration: -43% unburned NH3	Improved thermal efficiency, lower unburned ammonia, optimal trade-off between thermal efficiency and NOx	Higher NOx emissions, ANNs susceptible to getting trapped in local optimums
Zhu et al. (2025)	See Table 2	Efficient optimization of multiple conflicting objectives	Models possessed higher accuracy on training data than testing data (overfitting)
Goud and Baba (2026)	Optimal configuration obtained -10% CO, -45% UHC, -17% smoke opacity	Reported lower CO, UHC, and smoke opacity at the selected operating configuration	ANN superiority claim to conventional tools not directly verified
Björnsson and Tunestål (2024)	87.40%, 67.56%, & 69.85% accuracy classifying no-knock, medium-knock, heavy-knock, respectively. 74.5% overall accuracy for three-class knock classification	High accuracy in distinguishing between knock cases	Difficult differentiating combustions close to MAPO thresholds, still dependent on sensor data
Farhan et al. (2024)	See Table 4	Findings may be helpful toward ECU training and HCNG engine development	Only low intensity combustion conditions tested

Compiled from [3], [4], [6], [7], [9], [12], [13], [14]

Biographies

Dr. Raj Shah, is a Director at Koehler Instrument Company in New York, where he has worked for the last 25 plus years. He is an elected Fellow by his peers at ASTM, IChemE, AOCS, CMI, STLE, AIC, NLGI, INSTMC, Institute of Physics, The Energy Institute and The Royal Society of Chemistry. An ASTM Eagle award recipient, Dr. Shah recently coedited the bestseller, “Fuels and Lubricants handbook”, details of which are available at ASTM’s Long-awaited Fuels and Lubricants Handbook <https://bit.ly/3u2e6GY>. He earned his doctorate in Chemical Engineering from The Pennsylvania State University and is a Fellow from The Chartered Management Institute, London. Dr. Shah is also a Chartered Scientist with the Science Council, a Chartered Petroleum Engineer with the Energy Institute and a Chartered Engineer with the Engineering council, UK. Dr. Shah was recently granted the honorific of “Eminent engineer” with Tau Beta Pi, the largest engineering society in the USA. He is on the Advisory Board of Directors at SUNY Farmingdale (Mechanical Technology and Engineering Management), Auburn University (Tribology), and the State University of New York, Stony Brook (Chemical Engineering/Materials Science and Engineering). An Adjunct Professor at the State University of New York, Stony Brook, in the Department of Material Science and Chemical Engineering, Raj also has over 825 publications and has been active in the energy industry for over 3 decades.

Dr. Vikram Mittal, PhD is an Associate Professor in the Department of Systems Engineering at the United States Military Academy. His research interests include energy modeling, technology forecasting, and Alternative fuels. Previously, he was a senior mechanical engineer at the Charles Stark Draper Laboratory. He holds a PhD in Mechanical Engineering from MIT, an MS in Engineering Sciences from Oxford, and a BS in Aeronautics from Caltech. Dr. Mittal is also a combat veteran and a major in the U.S. Army Reserve.

Mr. Stephen Wang is an undergraduate mechanical engineering student at Rutgers, The State University of New Jersey. He is part of a thriving internship program at Koehler Instrument Company in Holtsville, NY under the supervision of Dr. Raj Shah.

Gavin Cunningham, EIT, is a Technical Applications & Sales Engineer at Koehler Instrument Company, Inc., where he supports the selection, application, and technical documentation of laboratory instrumentation for petroleum, fuels, lubricants, and related materials. He earned a Bachelor of Science in Chemical Engineering from the University at Buffalo and holds Engineer-in-Training certification in New York State. His technical interests include tribology, lubricant performance, fuel-quality analysis, laboratory automation, and the practical application of ASTM test methods in industrial and research laboratories.

Ms. Kate Marussich is part of a thriving internship program at Koehler Instrument Company in Holtsville, NY under the supervision of Dr. Raj Shah. Marussich is also a student in the department of Material Science and Chemical Engineering at Stony Brook University, where Dr. Shah serves on the External Advisory Board.

Ms. Prinika Kondoju is part of a thriving internship program at Koehler Instrument Company in Holtsville, NY, under Dr. Raj Shah. Kondoju is also a student in the department of Chemical and Biomolecular Engineering at the University of Massachusetts Amherst.

Ms. Fiona Njeri Okech is a member of a thriving petroleum research internship at Koehler Instrument Company, where she regularly contributes to the petroleum and energy research industry.



Vikram Mittal



Stephen Wang



Gavin Cunningham



Kate Marussich



Prinika Kondoju



Fiona Njeri Okech

Author Contact Details

Dr. Raj Shah, Koehler Instrument Company

- Holtsville, NY11742 USA
- Email: rshah@koehlerinstrument.com
- Web: www.koehlerinstrument.com



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5