



# EFFECT OF AI ON VARIOUS ALTERNATIVE FUEL TECHNOLOGIES

## Abstract

With the growing advancements in Artificial Intelligence, researchers are introducing innovative applications to combat the growing global demand for energy. For instance, researchers are aiming to make nuclear fuel safer and more efficient with AI assistance by reducing simulation times to anticipate potential failures quickly. Proton exchange membrane fuel cells, an expensive energy alternative, leverage AI-powered parameter optimization to make PEM fuel cells a more economically viable energy source, offering far greater efficiency and lower costs than traditional experimentation. Other sustainable sources, such as biodiesel, are benefiting from AI modeling and predictions that aid in efficiency optimizations and emission reductions. AI's increasing ability to tackle the complexity that plagues traditional theoretical models allows it to be applied to predict the low flammability limit of sustainable aviation fuel blends. Besides having a direct impact on fuel production, AI can be utilized to assist in creating infrastructure that enables sustainable habits to thrive.

## Introduction:

Artificial intelligence, or AI, is technology that simulates human intelligence, mimicking our abilities to solve problems, learn, and develop connections. Recently, AI has been growing rapidly with billions of dollars in private and government investment. In 2025, the US government allocated approximately \$11 billion in AI funding [1]. AI in the research field has been increasingly used for its powerful AI models which are programs trained with data to perform specific tasks. For instance, in the energy sector, AI models are being used to predict results that would have been unfeasible to do so with traditional complex models.

Alternative energy sources have been a focus over the past few

decades due to pressure to switch to more sustainable options, such as nuclear power, sustainable fuels, and hydrogen. Nuclear energy is when energy from the nucleus of atoms is harnessed through fission or fusion. Nuclear energy produces vast amounts of energy, with the trade-off of radioactive waste and questions about its safety. Sustainable fuel sources like Sustainable Aviation Fuel (SAF) and biodiesel are biofuels derived from biomass. Hydrogen Fuel Cells and hydrogen energy in general are expensive and difficult to synthesize. Hydrogen energy is chemical potential energy stored as hydrogen, which is then converted to water. This paper will examine how AI plays a role in all these different fuel types and how AI can boost sustainable fuel production and usage.

## AI in Nuclear Energy

In nuclear engineering, the behavior of systems, structures, and components regarding nuclear reactors is studied. Complex partial differential equations (PDEs) govern these physical models. Traditionally, we use tools like finite element analysis (FEA) simulations to break down the behavior of systems, structures, and components in real-life conditions into manageable variables, each governed by its own partial differential equation (PDE). By solving each PDE iteratively, each one builds upon the previously solved one to develop a cohesive model [2]. The resolution of these models depends on the time it spent processing information; the higher the resolution and the more intensive the calculations lead to more computational resources being used and the computing cost to increase. Currently, a possible solution is reduced-order modeling, where the dimensions of a complex model are simplified and linearized. This has proven to be useful but is limited by its inherent linearity. AI models have been rapidly developed as surrogates that overcome the limitations of simpler models, enabling the evaluation of both linear and non-linear functions. Researchers S.A. Cancemi et al utilize Convolutional Neural Networks (CNN) to model pellet-cladding interactions, an inherently complex finite element simulation, to improve the safety of nuclear plants [2]. Pellet cladding interaction occurs when the cladding of a pellet fails due to large power surges [3]. The cladding on the pellets serves as a crucial barrier, preventing radioactive materials within the pellets from escaping and contaminating the reactor [4]. In this experiment, a surrogate model (a simpler model of a more complex mathematical model) is introduced to predict the microstructural evolution and mechanical properties of AISI 316L stainless steel fuel cladding at different temperatures and radiation doses, thereby creating an accurate model that can be used to predict failures under various conditions.

CNNs are trained on a series of images and excel at image processing and pattern recognition. Images are passed through a hierarchy of "filters" where features are extracted. 13 parameters are included in this model: Mass density, Young's modulus, Poisson's ratio, Thermal expansion coefficient, Yield strength, Specific heat, Thermal conductivity, Shear modulus, Back stress for implicit creep, Yield stress for implicit creep, Specific heat, Centerline temperature, and Pressure [2]. These input features characterize materials and determine thermochemical behaviors. If we use a finite element model to simulate typical pressurized water reactor conditions, the FE fails to provide a real-time assessment of the cladding integrity on the pellet. However, the CNN surrogate model developed can offer rapid results (0.98 seconds) in predicting displacement, von Mises stress, and creep strain [2]. Displacement is the physical change of position of a point on an object (in this case, the pellet). Creep strain is the deformation that occurs (relative to time) due to high temperatures, and von Mises stress is used to

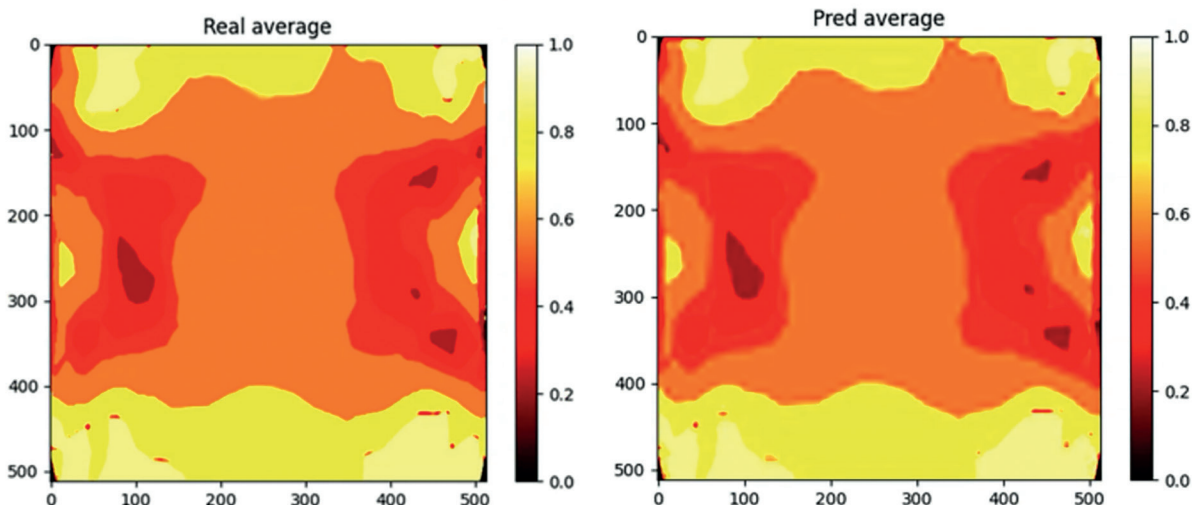


Figure 1: Real average von Mises stress of the pellet vs Predicted average von Mises stress from the CNN model [2].



predict material yielding under complex loading conditions [5]. The researchers determined that the CNN model is 17x faster than traditional Finite Element Analysis models, taking the FEA model 17.08 seconds to generate results [2]. These results show that the new CNN model is more efficient than traditional linear FEA models.

A total of 3,360 images were used to train Cancemi's model [1], which aimed to predict displacement, von Mises stress, and creep strain under given conditions. These images were generated using a finite element simulation depicting von Mises stress, creep strain, and displacement of the top, bottom, and side views under different conditions. The accuracy of the results produced was astonishing. Figure 1 displays the real average von Mises stress, compared to the predicted average von Mises stress [2]

The best performing models had a mean squared error of 0.000678 [2]. This indicates an extremely high level of accuracy for these models. The CNN model's highly accurate pattern recognition capabilities enable it to produce simulation results at a fraction of the time while maintaining traditional FEA model accuracy. Cancemi's study is extremely promising and is still in its early stages of development. These results demonstrate a significant reduction in processing time, with minimal compromise in error rates. With further research, pellet failures in nuclear reactors will be easier to predict and prevent, making nuclear energy a safer, more appealing, and cleaner alternative.

#### AI in Sustainable Aviation Fuel Blend

A previous study utilized a CNN surrogate model to simulate complex pellet cladding interactions, aiming to predict cladding failures. Another powerful AI model is an ANN model, or an Artificial Neural Network model. This model processes information through layers of interconnected nodes, mimicking how the human brain functions. The input data is analyzed, and subsequently, it is received by the hidden layer, which transforms the data through weighted connections and activation functions [6]. Finally, the model produces predictions or results. Researchers Z. Liu et al. trained an ANN model to cover the most significant classes of sustainable aviation fuel blends, aiming to accurately predict the low flammability limit (LFL) of fuel blends. LFL or the lowest fuel-gas mixture concentration that will facilitate a self-supported flame. In other words, the potency and efficiency of a fuel are better, the lower the flammability limit. The researchers fed the input matrix with data on the LFL of "drop-in fuel" which can be used as an immediate fuel alternative with no additional steps. The ANN model performed exceptionally well in predicting the LFL, as shown below, compared to other theoretical models. The blue dots (ANN LFL model) exhibit a strong correlation between the predicted and actual values, with

a total correlation coefficient of 0.994 [6]. The closer this value is to 1, the stronger the correlation.

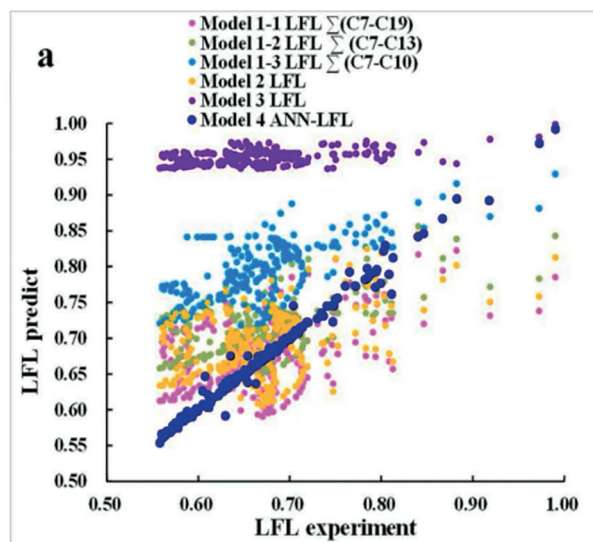


Figure 2: The correlation between predicted LFL values from multiple theoretical models and the experimental LFL values compared to the correlation shown by the ANN LFL model (blue) [6].

What makes Artificial Neural Networks so effective is that they can account for hidden, complex effects or layers by implementing artificial neurons. Some hidden complex effects include molecular structure and intramolecular and intermolecular forces. To avoid an overly complex model that would have resulted in a waste of resources, the researchers used the 43 most significant classes of hydrocarbons, which served as a surrogate for hydrocarbons with similar LFL within a 1% deviation. This model is so accurate that apparent deviations from traditional jet fuel values indicate that the fuel is "non-drop-in," meaning it cannot be used as jet fuel with modification.

Therefore, this is a potent tool that can be used to assess and design sustainable aviation fuels that meet the drop in fuel standards [6].

#### ANN in Biodiesel:

Currently, biodiesel accounts for 1% of the world's energy sources and is growing in number. Considering how much of our energy comes from petroleum derivatives (around 30% in 2024), we are quite a length away from replacing diesel with biodiesel [7], [8]. Biodiesel inherently cannot compete with the raw performance capabilities of diesel and faces issues in engine and cost efficiency. Researchers U. Rajak et al. built upon previous research regarding the effect of biodiesel-enriched diesel blends in direct injection of diesel engines. They plan to examine further the effects of engine speed on engine efficiency and emissions using ANNs. The use of AI circumvents the expensive and rigorous testing that comes with experimentation under specific constraints. The researchers initially conducted 75 trials consisting of different diesel and soybean biodiesel blends at different engine rpm. Simple tools were used to determine engine efficiency and emissions. These tools had a combined uncertainty of  $\pm 3.57$ . This uncertainty will most likely be reflected in the mean squared error (MSE) of the ANN model. The mean squared error is used as a value to determine the accuracy of a model; the closer it is to zero, the more accurate the model. Experimental data, along with data from databases, were then compiled and randomized. 70% of the data was used to train the ANN model, 15% to test, and the remaining 15% to validate. The model reported a mean squared error of 0.9 [7]. This series of training, testing, and validation was conducted to predict values for brake thermal efficiency, volumetric efficiency, CO<sub>2</sub> emissions, and NO<sub>x</sub> emissions. Both brake thermal efficiency and volumetric efficiency are crucial in determining an engine's overall efficiency. However, it is worth noting that the model's mean squared error for predicting CO<sub>2</sub> emissions was particularly low compared to the other models.

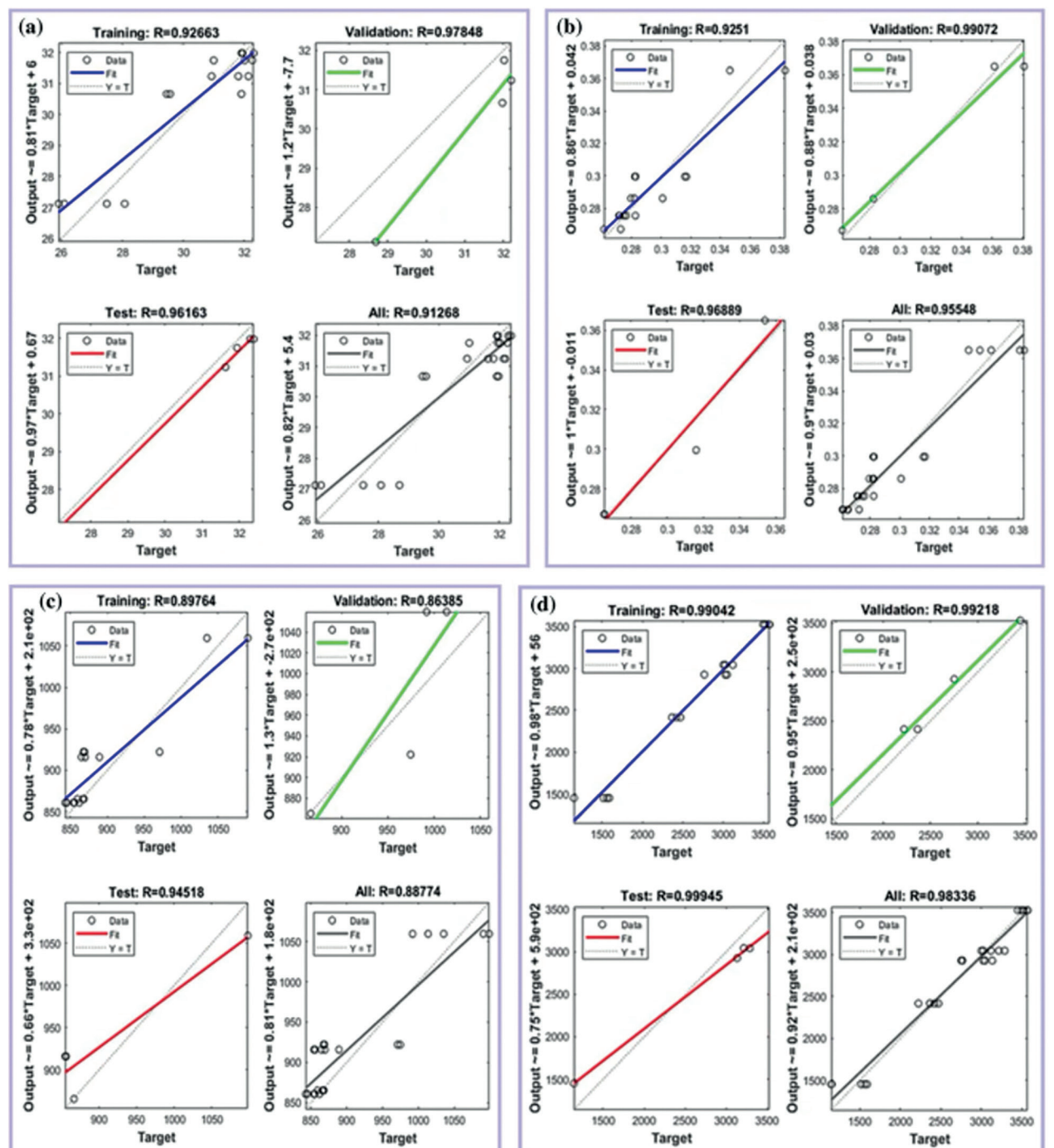


Figure 3 Training, Testing, Validating tests for a. BTE, b. VE, c. CO<sub>2</sub> Emissions, and d. NO<sub>x</sub> Emissions [7].

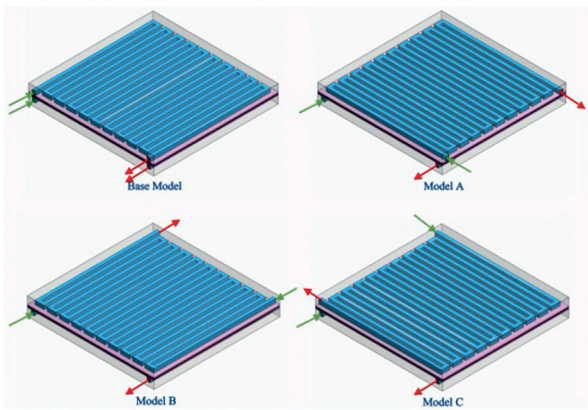


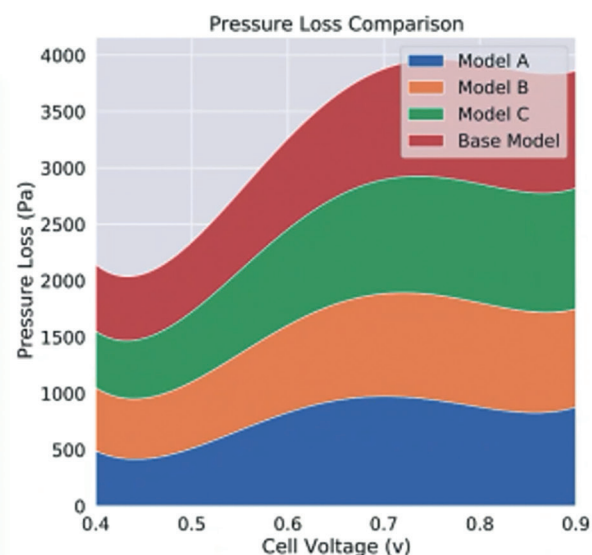
Figure 4 Shows the serpentine fuel cells, along with the 4 orientations in the trials [9].

Looking at Figure 3, the CO<sub>2</sub> emissions ANN model has an MSE of 0.888 in total, compared to the other model, which ranges from the high 0.90s to the low 0.90s, indicating either an issue within the artificial neural network itself or poor data quality [7]. BTE, or brake thermal efficiency, is one of the most highly valued indicators of engine performance. A high BTE results from a high caloric value and a high cetane number, both of which are key indicators of high-quality diesel. VE, or volumetric efficiency, is a reliable method for evaluating the success of fuel blends in a diesel engine. This parameter measures the ratio of the available volume in the cylinder and the intake of volume of air. BTE, VE, and emission ANN models are critical, especially regarding the more complex direct-injection diesel engines, which are far more efficient compared to their indirect injection counterparts. This study demonstrates how AI capabilities now extend to more nuanced and complex constraints, enabling the return of parameters based on multiple criteria.

**Artificial Intelligence in PEM Deep Neural Networks**

Proton exchange membranes (PEM) fuel cells are a promising alternative fuel source and a sustainable energy source. PEM fuels operate through an electrochemical process where hydrogen is converted into protons via a platinum catalyst. This chemical process results in only heat and water as byproducts, making it an immaculate process. However, the operating cost of this fuel cell is expensive, requiring high investments in platinum catalysts, which makes the energy produced expensive and unattractive. Researcher Ali Basem utilizes deep neural networks to optimize the parameters of PEM fuel cells, studying the fuel effect of flow orientation on power output to improve commercial availability. Basem builds off of previous innovations in PEM fuel cells, specifically serpentine channel fuel cells. This structure (seen in Fig. 5) has been proven to increase fuel cell performance significantly. The primary purpose of the deep neural network in this experiment is to predict additional points of the inlet humidity effect on output power. Initial data were analyzed from numerical simulations and validated through comparisons to previous studies. Then, a 4th-order polynomial regression is applied to the series of points generated by the deep neural network to derive a function that determines the optimal humidity to be at 14.57%. The lack of experimental study likely stems from the fact that it is a project undertaken by a single researcher, which may contribute to the low accuracy of the deep neural network model, at 87.53% [9].

This experiment studies three innovative flow orientations within



the serpentine architecture. In Figure 4, we can see the base model, model A (90°), model B (180°), and model C (270°) [9]. In each model, the flow direction has been shifted by increments of 90°. Multiphase simulations were conducted under multiple optimal parameters. In Figure 5, pressure loss and power consumption were measured at different cell voltages. Pressure loss is an issue where the ends of channels are unable to reach a proper pressure (around 1.0 atm), resulting in an imbalance of pressure within the system, which makes it challenging to obtain the correct cell voltage. Consumed power is the power consumed to output a specific voltage. The greater the required power, the lower the voltage. The results concluded that model A showed the lowest amount of pressure loss, and model C showed the lowest amount of power consumption for the demanded voltage.

Proton exchange membrane fuel cells remain financially unattractive, despite being beneficial, as they produce clean energy with minimal to no harmful byproducts. In this experiment, optimal operating parameters were determined to maximize specific characteristics of PEM fuel cells. The use of a deep neural network offers the potential for significant efficiency gains. The improvement in efficiency, however, was not enough to make PEM fuel cells more cost-efficient than other renewable energy sources, such as biofuels. However, the advancements highlighted in this experiment make PEM-fuel cell power increasingly likely.

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**AI-assisted refueling for hydrogen-powered vehicles**

The reality is that existing infrastructure limitations often hinder the implementation of innovative and novel technologies. A prime example of this is the increasing advancement of hydrogen-powered vehicles, a sustainable alternative to traditional gasoline vehicles. They are gaining popularity as new technologies continue to advance them. However, a limiting factor is the lack of refueling stations for fuel cell electric vehicles. Gasoline and diesel refueling stations are numerous and accessible, which makes it uncomfortable for electric cars to switch to fuel cells. Consumers often trade off their time and money when they switch to FCEV, ultimately ruining the consumer experience.

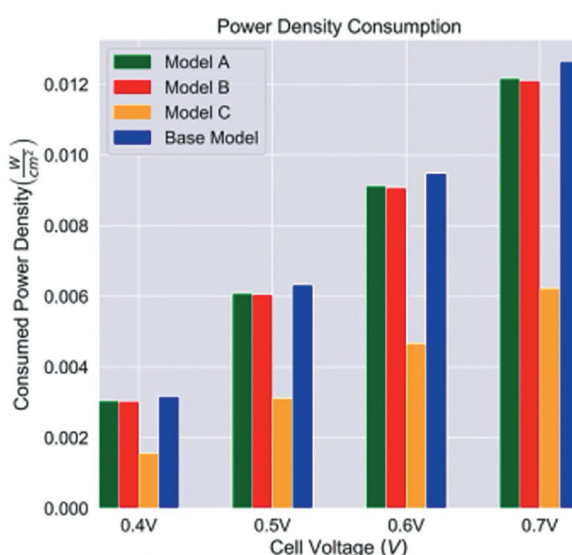


Figure 5 The graph on the left shows the pressure loss in the 4 different orientations, and the graph on the right shows the consumed power at 0.4 V, 0.5 V, 0.6V, and 0.7V [9]

Researchers S. Polymeni et al. utilized AI to enhance user experience and develop a cost-effective solution to optimize the refueling process. Their proposal is summarized as a model that predicts a vehicle's energy consumption using existing or predicted traffic data to determine optimal charging schedules and locations [10]. Energy consumption forecasts will inform the scheduling software that each driver should use based on destination and location, and when and where they should refuel.

The researchers implemented an autoregressive integrated moving average model (ARIMA). The ARIMA model has three components: the autoregressive component of the evolving variable of interest is based on past values, the integration component is based on differences in data values, and the moving-average component is based on past errors. The ARIMA model is designed to predict future points in a time series. In this experiment, it is utilized to predict energy consumption.

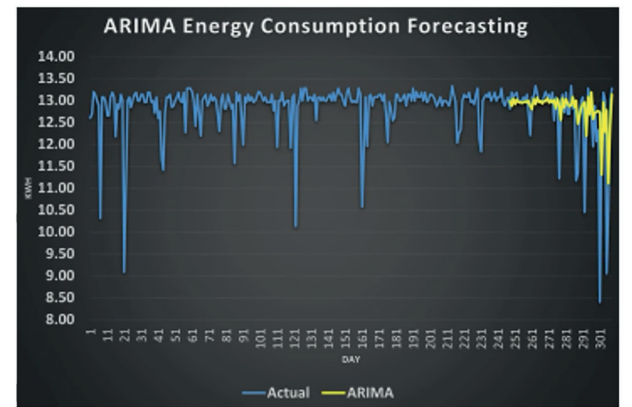


Figure 6 Comparison of ARIMA-predicted fuel consumption and Actual fuel consumption [10].

Looking at Figure 6, the results are surprisingly accurate, considering the ambitious nature of this goal. Predicting the future based on statistics and probability is a challenging task, as it is impossible to fully model randomness. The values are accurate to the extent that they are much higher than the actual values. This poses issues, as energy consumption forecasting aims to optimize the refueling process by carefully scheduling individual drivers to avoid frustrating long queue times. This prediction could optimize the process to an extent, but it can never fully achieve complete optimization. This experiment is excellent proof of concept, as the idea faces other limitations. If faced with large fleets of vehicles, the data processing and infrastructure requirements would overload this process, leading to prolonged process times and a resurgence of the infrastructure issue.

**Conclusion:**

Artificial Intelligence and its capabilities continue to grow year by year. With those innovations come novel applications in nuclear energy, hydrogen fuel cells, biodiesel, and sustainable aviation fuel. AI's applications range from faster simulation of complex phenomena to predicting fuel characteristics from input data. AI's applications only accelerate the advancement of fuel technology, making it quicker and cheaper. Despite this, AI still faces challenges regarding accuracy and computing power. Our current processing units are expensive and demanding, while complex neural networks provide highly accurate results; others do not. However, the role of Artificial Intelligence in society continues to grow as more funding is poured into this field. With further advances in neural network models, optimizations, and improvements that would have taken years of experimental trials are now achieved in seconds, accelerating advancements to new heights.

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### 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, ASTM,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 "Eminent engineer" with Tau beta Pi, the largest engineering society in the USA. He is on the Advisory board of directors at Farmingdale university (Mechanical Technology), Auburn Univ (Tribology), SUNY, Farmingdale, (Engineering Management) and State university of NY, Stony Brook (Chemical engineering/ Material 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 700 publications and has been active in the energy industry for over 3 decades.



Clark Ye

**Mr. Clark Ye** is part of a thriving internship program at Koehler Instrument Company in Holtsville, NY underneath Dr. Raj Shah. Ye 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.

**Mr. Gavin Thomas** is part of a thriving internship program at Koehler Instrument Company in Holtsville, NY and is a recent graduate of the Chemical and Molecular Engineering program at Stony Brook University. He also works as a process engineer at Mill-Max in Oyster Bay, NY where he becomes hands-on with various production processes to ultimately improve safety, efficiency, and cost-effectiveness.



Gavin Thomas

### Author Contact Details

**Dr. Raj Shah, Koehler Instrument Company**

- Holtsville, NY11742 USA
- Email: [rshah@koehlerinstrument.com](mailto:rshah@koehlerinstrument.com)
- Web: [www.koehlerinstrument.com](http://www.koehlerinstrument.com)

