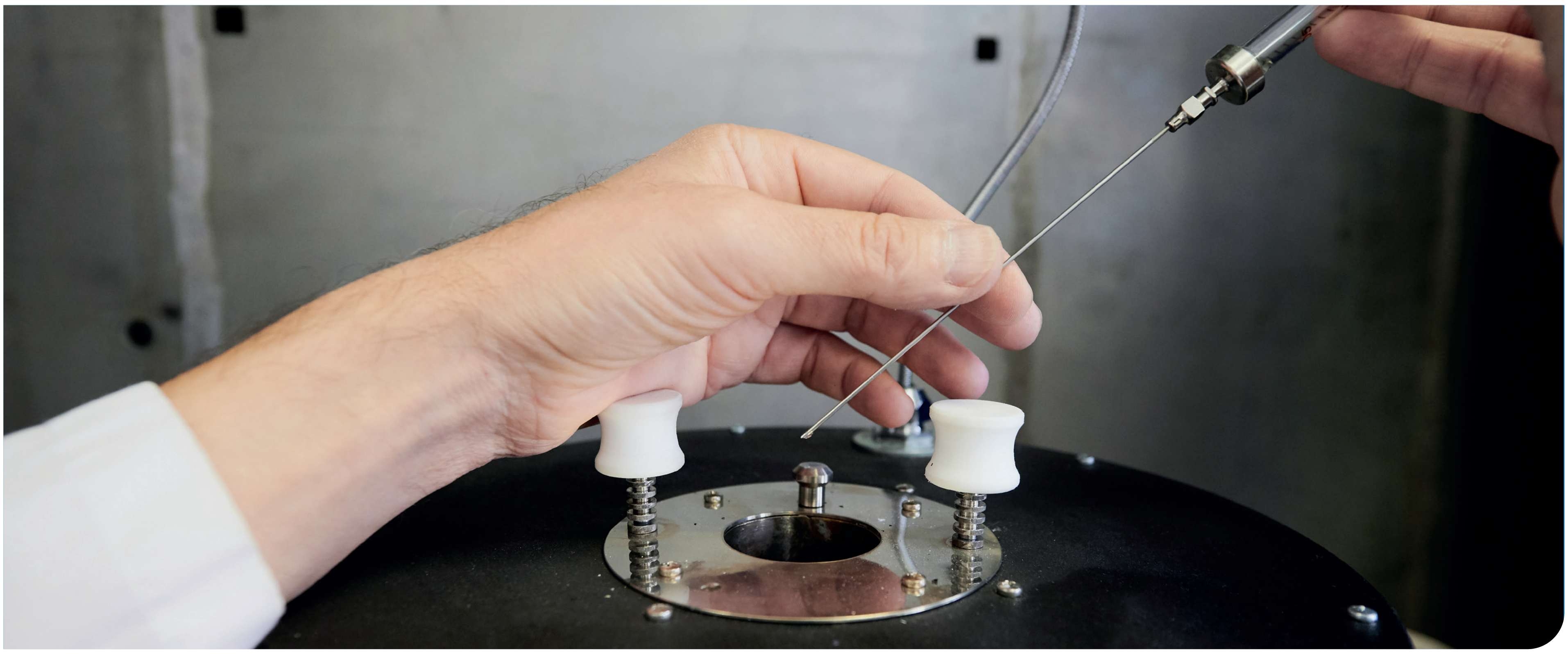
UPDATES AND ADVANCEMENTS IN OCTANE TESTING



Introduction:

The automobile is a revolutionary invention that requires no further introduction. Equally as impactful was its subsequent popularization of gasoline. However, its discovery in 1859 was uneventful, as it was discarded as a byproduct of crude oil refining[1]. It would remain as such until the invention of automobile engines in 1892, which required gasoline as its primary fuel source[2]. By the 1920s, millions of gasoline-powered cars populated the United States. Moreover, an equal number of gasoline service stations opened up across the nation[1]. To this day, gasoline continues to dominate automotive fuel[3], and countless developments in gasoline production and its refinery have ensured that the fuel keeps pace in potency and efficiency with the industries it powers.

One of the most significant testing procedures for gasoline is the Octane test, also known as the engine knock test[4]. In this test, gasoline blends are measured for their propensity to knock. Knock occurs from the premature combustion of the air-fuel mixture in an internal combustion engine, leading to undesirable and damaging high-pressure shock waves and a characteristic knocking sound[5]. Octane tests and their numbers hold significant value to the refinement and efficacy of gasoline as a whole. And though people likely do not understand the intricacies of octane testing, car owners are guaranteed to understand the octane numbers on gasoline pumps. This paper illustrates the importance and relevancy of both octane testing and octane numbers, noting the process's unique strengths and discussing several recent advancements that hold positive implications for future octane engine testing.

Octane Ratings, and Octane Testing:

Firstly, it is important to define keywords and processes before elaborating further. All forms of gasoline are assigned an octane rating (AKA octane number), typically seen in gas pumps such as Figure 1, with higher octane ratings indicating more stable fuels[6]. Octane numbers are an average of two octane rating methods: Motor Octane Number (MON) and Research Octane Number (RON). RON is a measure of the gasoline's performance in gentler conditions (around 600 rpm and intake air at 49℃)

Figure 1: Three octane numbers differentiating three different gasoline types of varying stability [9].

whereas MON is the gasoline's performance in more intensive conditions (around 900 rpm and intake air at 149℃)[7], and octane testing is a process by which both numbers and the gasoline's overall octane rating is measured and determined. Octane testing is a theoretically simple process. In a specialty CFR engine, the fuel is observed under standardized operating conditions. The compression ratio of the engine is then increased, which in turn increases the pressure and temperatures during combustion, hence increasing the propensity of a fuel to knock. When the engine knocks at a certain intensity, the associated compression ratio is then compared to a reference fuel blend of iso-octane and n-heptane, which knocks at the same intensity for the compression ratio. The octane number of the fuel is the blend of iso-octane in that fuel[8]. Then, relating to the reference fuels, the specific RON or MON of the fuel is determined as conditions for the tests differ in engine speed and idle air temperatures[6]. With both ratings determined, the octane number posted on fuel pumps is given as the average of the RON and MON.

As mentioned, octane testing for MON and RON are two separate processes. Therefore, separate testing machines are employed, each configured toward separate tests. Current devices allow RON and MON tests on the same engine, but many scientists still prefer using separate machines tailored to each[6]. To consolidate research efforts, the American Society for Testing Materials (ASTM) has designated standards for both testing processes, among many others. As such, this paper will refer to RON and MON testing by their designated method names: ASTM-D2699 for RON testing of engine fuel, and ASTM-D2700 for MON testing of engine fuel[10].

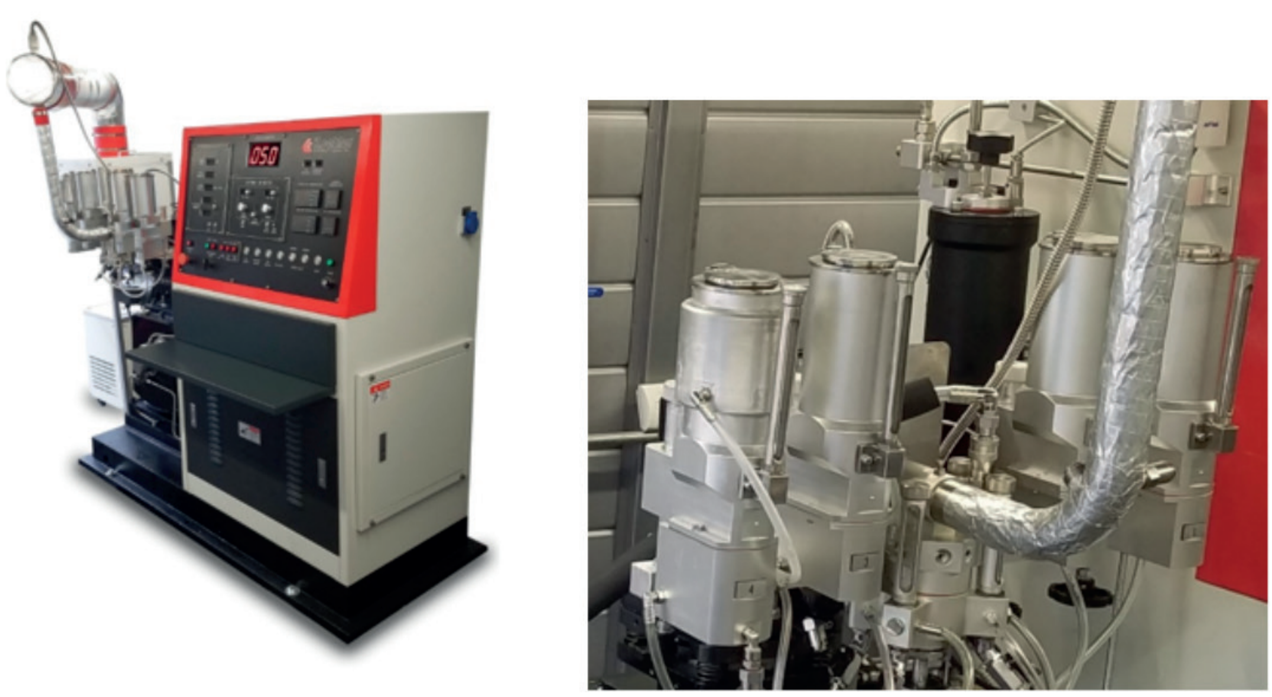


Figure 2: A combination octane rating unit engine octane. This unit (left) is able to determine both MON and RON values. Due to the nature of the device, both tests can be operated using the same chamber. A close-up of the carburetor is shown (right)

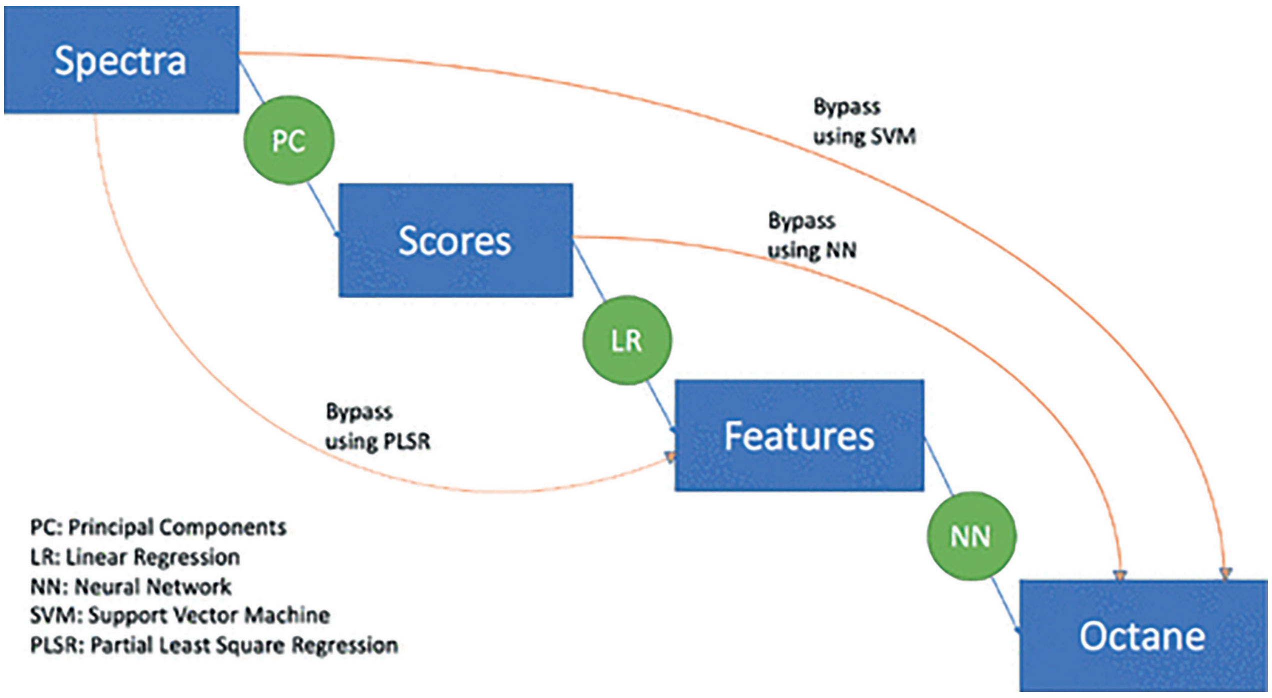


Figure 3: A model of the road map for the experiment 13.

Importance and Relevance of Octane Testing:

With names and definitions properly defined, we must now ask why it is so important to continue octane testing development. Fundamentally, octane numbers represent the stability of gasoline and its tendency against knocking. A high octane number indicates a more stable fuel and thus a lower chance of auto ignition during use[6]. By accurately rating the octane quality of fuels in such a way, researchers and consumers alike can gauge the efficacy of many different fuels. As oil companies distill the number to simply imply the quality of gasoline, drivers benefit passively from the association of higher octane numbers to higher quality fuels[6].

From a researcher's standpoint, octane numbers also hold relevance. Measuring an accurate octane rating serves as a valid marker for retracing the creation of that fuel. With exact samples, recreating a successful octane fuel process can be much clearer given a numerical value that resulting compounds must also match. In addition to boosting the consistency of samples, future research building on potential compounds will have a more solid foundation with a traceable pathway towards producing that compound.

Finally, the simplest benefit of all would be the overall efficiency of the engine. While the act of reducing knocking is itself a boon to efficiency, further research has determined a link with the sensitivity of fuel, the difference between the RON and MON values, and the engine's efficiency[11]. In a remarkable study conducted in 2005 by a team from Shell Global Solutions on the concept, the group discovered a positive association between increasing the RON and subsequent sensitivity of the fuel and the engine efficiency and fuel consumption, with sensitivity more strongly influencing energy efficiency at lower RON values (92) than higher values (98)[11]. Therefore, by upholding a higher sensitivity (i.e. a lower MON for a given RON), fuels can have increased anti-knock performance. Octane number testing continues to lead the industry, and its importance cannot be understated. Without it, fuel research would be decades behind, and fuel efficiency would not be as high as it is today.

Recent Innovations:

Like all scientific innovations, octane testing has experienced a myriad of different innovations to improve the process. As octane numbers are a rather significant factor in fuel and can only be determined experimentally[6], many researchers have devised methods of predicting octane numbers and other qualities by extrapolating data from previous research to make the rating process easier. This paper will cover several recent advancements in the area of octane research, making note of their significance and positive implications on future octane testing.

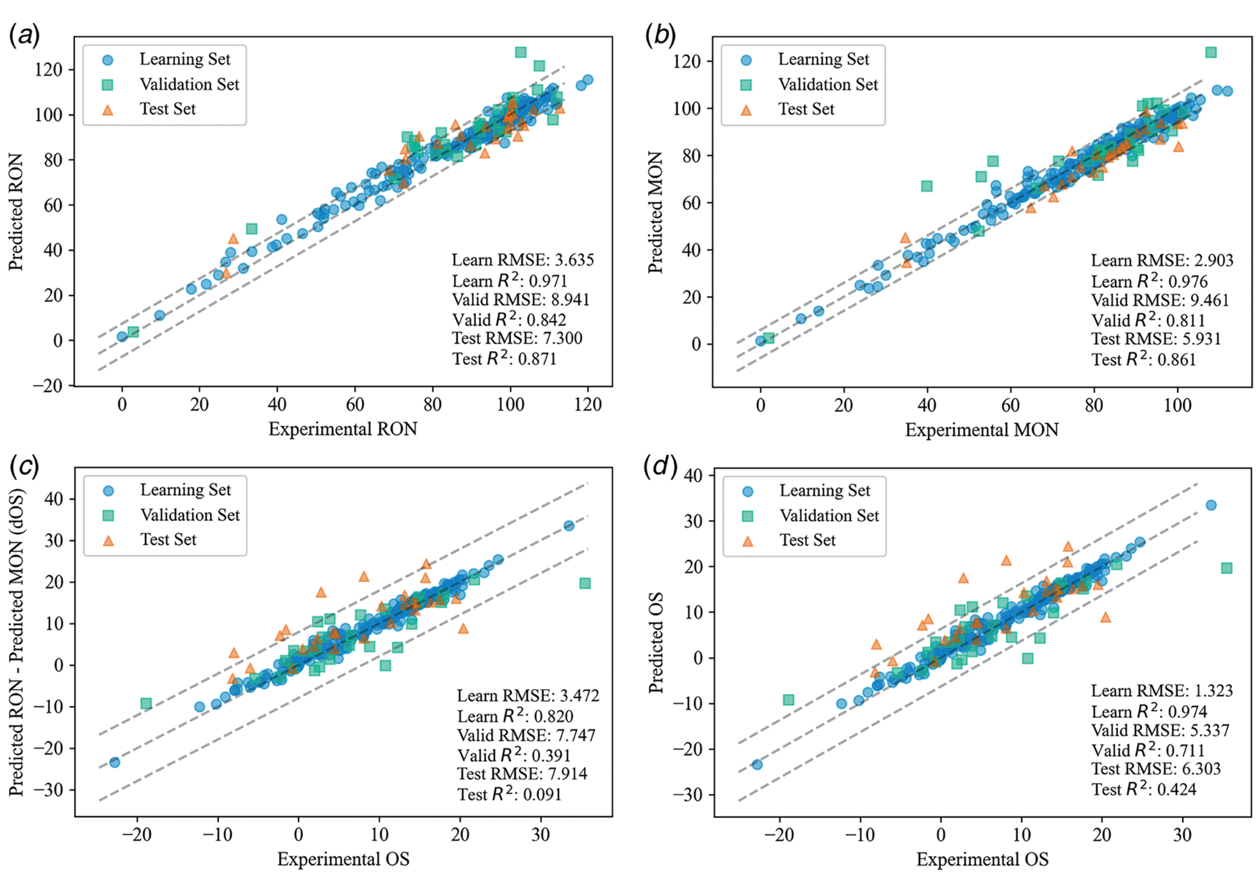


Figure 4: Plots of individual ANNs showing predicted vs experimental values for ROR (RON), MOR (MON), dOS, and OS[14].

Infrared Spectroscopy:

Firstly, a research group from the King Abdullah University of Science and Technology in Saudi Arabia produced a model for predicting RON and MON using infrared spectroscopy (IR) of pure components[13]. The area of fuel property predictions is extensive, as direct testing using proper equipment would be far too costly and impractical to conduct[13]. An area of study in this field relates to chemometric-based fields areas of research, applying the partial least-squares regression (PLSR) algorithm to predict octane numbers. However, new approaches such as artificial neural networks (ANNs) have become increasingly more prominent as they have proven to accurately predict molecule behaviors and other qualities within the compound. To acknowledge the prevalence of ANNs, the group explored several methods of gas-phase IR spectra of hydrocarbons and ethanol to predict the molecular properties of their compound. Then, the team applied its findings to an ANN to demonstrate IR spectroscopy's viability in octane number prediction. According to the study, the IR spectra of 61 pure hydrocarbon species were employed to create 148 blends of hydrocarbons[13]. Then, the data for each species was collected and run through various algorithms. Either principle component analysis (PCA) or singular value decomposition (SVD) was used to simplify the data, and PLSR was used to derive features from the IR spectra.

From the results, the study concluded that the model was a success. The group was able to extract the necessary data to predict the efficacy of the compound from IR spectra and PLSR. Furthermore, the team also demonstrates the use of ANN to better capture octane behavior, capturing errors well within the margin of error for RON and MON values[13]. Thus, the efficacy of IR spectroscopy as a method of octane number prediction is a rousing success, allowing for future models to be produced using the IR spectra of pure hydrocarbons and other components.

Artificial Neural Networks:

Advancing a method mentioned in the previous study, a 2023 study conducted by a research group from the University of Massachusetts illustrates an approach to developing a model that predicts octane number and octane sensitivity using ANNs[14]. As previously mentioned, physical octane testing for large sets of potential fuels would be a waste of time, money, and samples. Therefore, this team employed ANNs, which are effective at predicting the properties of molecules without the need for physical samples[14]. These networks are trained with quantitative structure-property relationship (QSPR) descriptors, which inform properties of single-component fuels such as octane and have the unique potential to capture fundamental properties and interactions that would be lost with other datasets. For modeling combustion-related properties of hydrocarbons, numerous methods exist using many other approaches for modeling. Still, research has proven that ANNs have outperformed other models when concerning prediction accuracy of the final product[15]. Furthermore, ANNs have previously been used to predict RON and MON values of gasoline and gasoline blends with great success[16]. The study then proposes two different methods for predicting the octane sensitivity (OS) of a given compound: either by predicting RON and MON individually to compute the OS or by cutting out the middleman and directly computing the OS. Afterwards, in both cases, ANNs were trained on the relevant descriptors, and the fuel properties of 278 unique compounds were predicted for both methods.

These results from the experiment were astounding and impactful. From a direct analysis of the data, the ANNs predicted the RON, MON, and OS values effectively, with set percentage errors falling within acceptable measures, as shown in Figure 4[14]. Given such percentages, the study concluded that the models performed more effectively when directly predicting OS rather than predicting the individual RON and MON values, as the general error value when computing OS is smaller in comparison to computations performed with two values possessing errors. In addition to their fairly accurate predictions, the models were able to identify the exact origins of reactivity within the molecule's structure[14], as the QSPR descriptors allow for fundamental insights into the properties responsible for molecule reactivity. Finally, the ANNs in the study successfully identified hidden relationships between molecular structure and reactivity, highlighting several high-potential molecular fuels that are currently being studied as viable sources. Needless to say, the artificial neural network models were a complete success, and the information contained within the QSPR descriptors provides an incredibly strong foundation for the future chemical analyses of octane fuels.

Conclusion:

To conclude, octane testing is a vital part of gasoline manufacturing. Analyzing octane ratings not only informs the overall energy efficiency of the fuel but also improves the efficiency of further octane developments. In attempting to synthesize higher octane ratings, researchers have regularly innovated on its components, developing new methods of increasing efficiency and prediction models to discover hidden fuel sources and further advance the growth of fuels. Undoubtedly, octane testing will remain significant for decades to come, as new fuels are discovered and octane ratings continue to grow.

Table 1: The ten most influential QSPR Descriptors for OS, their importance, and description [14].

DESCRIPTOR NAME	IMPORTANCE	DESCRIPTION
AVS_B(s)	0.0380	Average vertex sum from Burden matrix weighted by I-state
nCsp2	0.0344	Number of sp^2 hybridized carbon atoms
SIC1	0.0272	Structural information content index (neighborhood symmetry of first-order)
Chi_Dz(p)	0.0268	Randic-like index from Barysz matrix weighted by polarizability
CIC1	0.0250	Complementary information content index (neighborhood symmetry of first-order)
SpMax1_BH(s)	0.0228	Largest eigenvalue n. 1 of Burden matrix weighted by I-state
SpMax1_B(s)	0.0225	Largest eigenvalue from Burden matrix weighted by I-state
Eta_D_epsiB	0.0202	Eta measure of unsaturation
Chi1_EA(ed)	0.0164	Connectivity-like index of order one from edge adjacency mat. weighted bt edge degree
LLS_01	0.0161	Modified lead-like score from Congreve et al. (six rules)

Resources:

1. U.S. Energy Information Administration. "Gasoline Explained. History of Gasoline." [Online]. Available: https://www.eia.gov/energyexplained/gasoline/history-of-gasoline.php
2. Thoughtco. "History of Gasoline." [Online]. Available: https://www.thoughtco.com/history-of-gasoline-1991845
3. The Global Economy. "Gasoline Consumption - Country Rankings." [Online]. Available: https://www.theglobaleconomy.com/rankings/gasoline_consumption/
4. Intertek. "Octane Testing." [Online]. Available: https://www.intertek.com/petroleum/testing/octane/
5. Department of Engineering Science. "Knock and Auto-Ignition Study in Spark Ignition Internal Combustion Engines." [Online]. Available: https://eng.ox.ac.uk/tpsrg/research/thermal-propulsion-systems/knock-and-auto-ignition-study-in-spark-ignition-internal-combustion-engines/
6. U.S. Energy Information Administration. "Gasoline Explained. What is Octane." [Online]. Available: https://www.eia.gov/energyexplained/gasoline/octane-in-depth.php
7. Leal, A., Martins, F.G. 2018. "Motor Octane Number." Science Direct. [Online]. Available: https://www.sciencedirect.com/topics/engineering/motor-octane-number
8. Petro Online. "What is Octane Testing?"[Online]. Available: https://www.petro-online.com/news/analytical-instrumentation/11/breaking-news/what-is-octane-testing/56073
9. Mental Floss. "What do the Numbers on Gas Pump Buttons Mean?" [Online]. Available: https://www.mentalfloss.com/article/655334/what-do-numbers-gas-pump-buttons-mean
10. Sinpar Petroleum Testing Equipment. "What are ASTM D2700 and ASTM D2699?" [Online]. Available: https://www.sh-sinpar.com/what-are-astm-d2700-and-astm-d2699.html
11. Prakash, A., Wang, C., Janssen, A., et al. "Impact of Fuel Sensitivity (RON-MON) on Engine Efficiency," SAE Int. J. Fuels Lubr. 10(1):2017, doi: 10.4271/2017-01-0799. [Online]. Available: https://www.semanticscholar.org/paper/Impact-of-Fuel-Sensitivity-(RON-MON)-on-Engine-Prakash-Wang/c7252d67e9077f32d60e71dd0dd2e52014d2f24c
12. Sinpar Petroleum Testing Equipment. "How to Test Gasoline Octane." [Online]. Available: https://www.sh-sinpar.com/how-to-test-gasoline-octane-knock-test-engine.html
13. Al Ibrahim, E., Aamir, F. "Octane Prediction from Infrared Spectroscopic Data." Energy & Fuels, vol. 34, no. 1, 2020, pp. 817–26, https://doi.org/10.1021/acs.energyfuels.9b02816. [Online]. Available: https://pubs.acs.org/doi/10.1021/acs.energyfuels.9b02816

About the Authors

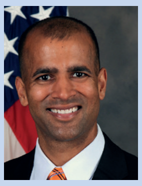
Dr. Raj Shah is a Director at Koehler Instrument Company in New York, where he has worked for the last 28 years. He is an elected Fellow by his peers at IChemE, CMI, STLE, AIC, NLGI, INSTMC, Institute of Physics, The Energy Institute and The Royal Society of Chemistry. An ASTM Eagle award recipient, Dr. Shah recently coedited the bestseller, "Fuels and Lubricants handbook", details of which are available at ASTM's Long-Awaited Fuels and Lubricants Handbook 2nd Edition Now Available (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 honourific of "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 575 publications and has been active in the energy industry for over 3 decades. More information on Raj can be found at https://bit.ly/3QvfaLX

Contact: rshah@koehlerinstrument.com

Mr. Beau Eng is part of a thriving internship program at Koehler Instrument company in Holtsville, and are students of Chemical Engineering at Stony Brook university, Long Island, NY where Dr.'s Shah and Mittal are on the external advisory board of directors.

Beau Eng

Dr. Vikram Mittal, is an Associate Professor at the United States Military Academy in the Department of Systems Engineering. He earned his doctorate in Mechanical Engineering at the Massachusetts Institute of Technology where he researched the relevancy of the octane number in modern engines. His current research interests include various energy technologies, system design, model-based systems engineering and modern engine technologies. He has numerous publications in various peer reviewed journals.



Vikram Mittal

14. SubLaban, A., Kessler, T., Dam, N., et al. "Artificial Neural Network Models for Octane Number and Octane Sensitivity: A Quantitative Structure Property Relationship Approach to Fuel Design." Journal of Energy Resources Technology, vol. 145, no. 10, 2023, https://doi.org/10.1115/1.4062189. [Online]. Available: https://asmedigitalcollection.asme.org/energyresources/article-abstract/145/10/102302/1160263/Artificial-Neural-Network-Models-for-Octane-Number?redirectedFrom=fulltext
15. Kessler, T., St John, P., C., Zhu, J., et al. "A Comparison of Computational Models for Predicting Yield Sooting Index." Proc. Combust. Inst., 38 (1), pp. 1385–1393. [Online]. Available: https://www.sciencedirect.com/science/article/abs/pii/S1540748920301784
16. Van Leeuwen, J. A., Jonker, R. J., Gill, R. "Octane Number Prediction Based on Gas Chromatographic Analysis With Non-Linear Regression Techniques," Chemom. Intell. Lab. Syst., 25 (2) 1994, pp. 325 –340. [Online]. Available: https://www.sciencedirect.com/science/article/abs/pii/0169743994850518

Author Contact Details

Dr. Raj Shah, Koehler Instrument Company • Holtsville, NY11742 USA • Email: rshah@koehlerinstrument.com • Web: www.koehlerinstrument.com