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In-line monitoring of base oil properties in refinery operations using process Raman spectroscopy

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Abstract

Base oils, classified into Groups I–V, serve as the foundations for lubricant formulations, with each group offering distinct compositions and performance characteristics. Ensuring accurate insight into base oil properties is essential for optimizing blend ratios, maintaining product quality, and meeting operational efficiency targets. Process Raman spectroscopy enables real-time, non-destructive measurement of these properties directly in the production environment, reducing reliance on time-intensive laboratory methods and supporting continuous process control. This study demonstrates the capability of the Thermo Scientific™ MarqMetrix™ All-In-One Process Raman Analyzer to quantify 17 critical base oil quality attributes using chemometric modeling and automated deployment through the RunSpex platform. The models delivered strong correlation and repeatability across boiling range, viscosity, volatility, and compositional metrics. These results validate process Raman as a scalable, in-line process monitoring solution that enhances production efficiency, enables predictive maintenance, and strengthens refinery decision-making.

Introduction

Base oils are the building blocks of lubricants. Base oils are split into five main groups (I – V). The groups vary based on their refining process, chemical composition, and performance characteristics. Group I oils are solvent-refined, containing higher levels of sulfur and unsaturated hydrocarbons, while Group II oils are hydrocracked, offering better oxidation stability. Group III oils undergo severe hydrocracking or hydro isomerization, resulting in very low sulfur content and a high viscosity index. Group IV oils are chemically synthesized polyalphaolefins (PAOs), known for their superior performance in extreme conditions. Group V includes all other base oils, such as esters and polyalkylene glycols, used for specialized applications.

The base oils are combined in various ratios and quantities to produce lubricants used for a wide array of applications, from automotive engines to industrial machinery. This means actionable information about the base oil properties is vital to ensure the right quantities are blended to reach the desired end lubricant product. Proper blending ensures optimal performance, cost-effectiveness, and compliance with specific application requirements and regulatory standards.

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Process Raman spectroscopy offers the capability to deliver necessary measurements of the base oils in real time without sample handling, all within a small footprint. This non-destructive analytical technique uses the scattering of light to provide detailed information about the molecular composition and structure of the base oils. One of the significant advantages of process Raman spectroscopy is its ability to provide continuous monitoring and enable potential control of the base oils, allowing for optimal production of lubricants with the desired properties. Traditional methods of base oil (and lubricant) analysis often require sample collection and laboratory testing, which can be time-consuming and may not provide real-time data. In contrast, Raman spectroscopy can be integrated directly into the industrial process, offering immediate feedback on condition and performance. This real-time monitoring allows for prompt adjustments and interventions, ensuring that the lubricants maintain their desired properties and perform optimally. In addition to real-time monitoring, process Raman spectroscopy can also provide valuable data for predictive maintenance. By continuously tracking the properties of base oils, it is possible to identify trends and potential issues before they lead to the production of out-of-spec material.

A key advantage of the MarqMetrix All-In-One Process Raman Analyzer system is its measurement flexibility, made possible through a range of sampling optics. This adaptability enables seamless transfer of analysis from the laboratory to the industrial process with minimal effort or disruption. By accommodating diverse sample types and operating environments, the system delivers versatile, real-time insights where they are needed most.

This application note demonstrates the use of the MarqMetrix All-In-One Process Raman Analyzer for the measurement of 17 base oil quality properties.

Experimental

Approximately 250 samples of group II and group II base oils were analyzed using a MarqMetrix All-In-One Process Raman Analyzer. The samples were collated with the appropriate reference data and processed using chemometrics data analysis methods. The resulting models were then deployed into RunSpex, a software platform onboard the MarqMetrix All-In-One Process Raman Analyzer, for real-time analysis and monitoring of process data. This deployment allowed for continuous and automated analysis of the samples, providing immediate feedback and insights.

Results and discussion

Table 1 presents the results generated by the chemometrics model for each base oil property along with the corresponding ASTM method. Each property exhibited a strong correlation between the measured and predicted values, indicating the models' accuracy and reliability. This excellent correlation demonstrates the applicability and robustness of the MarqMetrix All-In-One Process Raman Analyzer approach for quality measurements of lubricants. By accurately predicting the properties of interest, the methods prove to be a valuable tool in ensuring the consistency and performance of base oils. These findings highlight the potential of the MarqMetrix All-In-One Process Raman Analyzer for in-line monitoring of the base oil quality in the refinery, providing a reliable means of maintaining product standards.

Property	Number of samples	R^2	Model accuracy	Range	ASTM method
Initial Boiling Point (IBP) (°F)	246	0.99	5.92	506 - 758	D86
T05 (°F)	246	0.99	4.02	560 - 822	
T10 (°F)	246	0.99	3.72	575 - 852	
T15 (°F)	246	0.99	3.60	584 - 871	
T20 (°F)	246	0.99	3.51	592 - 886	
T30 (°F)	246	0.99	3.57	605 - 908	
T50 (°F)	246	0.99	3.66	626 - 942	
T70 (°F)	246	0.99	3.75	648 - 978	
T80 (°F)	246	0.99	4.85	656 - 1020	
T90 (°F)	246	0.99	6.71	672 - 1068	
T95 (°F)	246	0.99	6.17	683 - 1073	
FBP (°F)	246	0.99	8.87	710-1092	
Viscosity @ 40°C	246	0.99	1.42	9.5 – 126.5	D445
Viscosity @ 100°C	246	0.99	0.11	2.4 – 12.7	
Pour Point	190	0.93	3.08	-51 - -9	D97
Noack Volatility	70	0.97	0.63	7.3 – 19.4	D5800
Aromatics	187	0.91	0.18	0 – 2.3	D2007

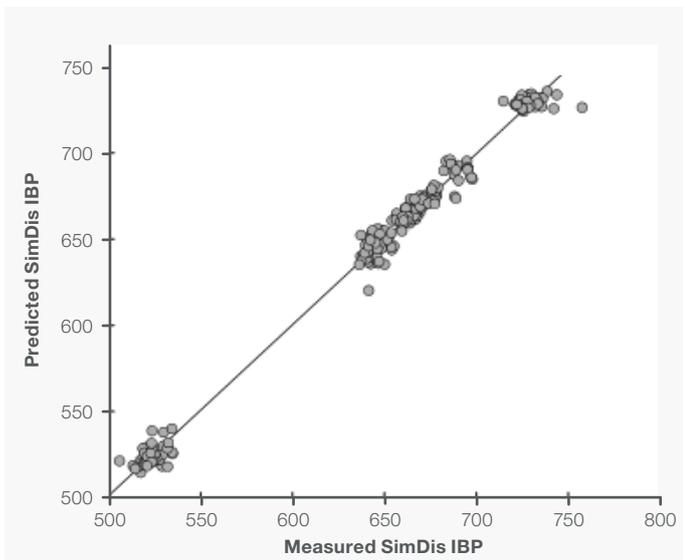Table 1. Prediction of lubricant properties.

Figure 1. IBP Simulated distillation (SimDis) model.

Simulated Distillation (SimDis) is a vital analytical technique widely used in the oil and gas industry. It is the primary method for determining the boiling point distributions of lubricants, which is essential for assessing their quality and compositional makeup. Figure 1 illustrates the output from SimDis models. Real-time prediction of SimDis results provides critical insights into the process and the resulting lubricants, which might be overlooked in a standard SimDis analysis that can take up to 60 minutes.
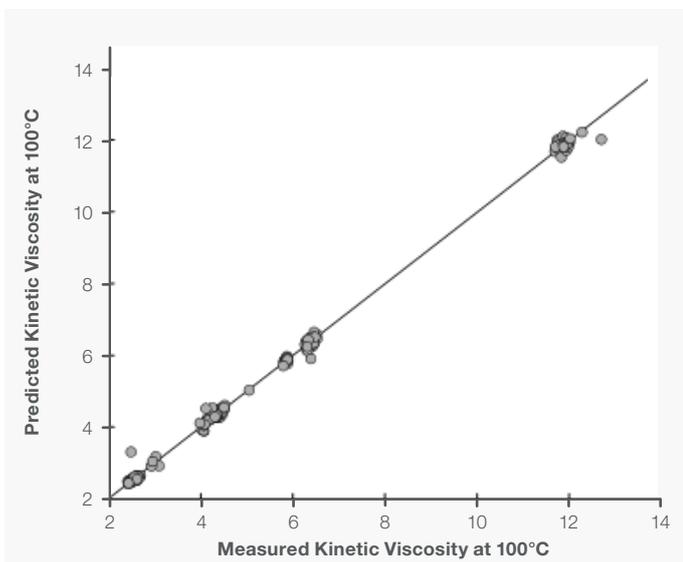

Figure 2. Kinetic viscosity model.

Kinematic viscosity is a critical quality parameter for lubricants, as it measures how easily the lubricant will flow at specific temperatures. Accurate measurement of kinematic viscosity is essential for ensuring optimal lubricant performance and stability. The process Raman was utilized to measure the kinematic viscosity at 40°C and 100°C. The results (Figure 2) showed a high degree of correlation and accuracy, demonstrating that the MarqMetrix All-In-One Process Raman Analyzer is capable of precisely quantifying the kinematic viscosity of lubricants. This capability ensures reliable assessment and helps in maintaining the desired performance characteristics of the lubricants under various operating conditions.
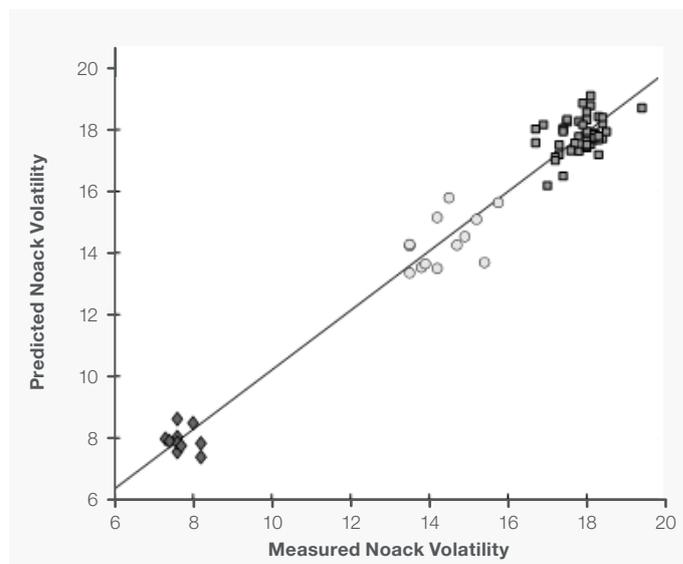

Figure 3. Noack volatility predictive model.

Noack volatility is a measure of an oil's tendency to evaporate at high temperatures. Lubricants with high Noack volatility can experience greater evaporation at elevated temperatures, which can negatively impact their performance and chemical stability. Assessing Noack volatility is crucial for determining the quality and future performance of the base oils. Figure 3 illustrates the resulting model for measuring Noack volatility. The models demonstrate a high degree of correlation and accuracy, enabling rapid assessment and quantification of Noack volatility using a MarqMetrix All-In-One Process Raman Analyzer.

Property	A			B		
	Mean value	StDev	RC	Mean value	StDev	RC
IBP (°F)	646	1.4	3.9	728	2.0	5.7
T05 (°F)	701	0.6	1.6	800	0.9	2.4
T10 (°F)	727	0.6	1.7	839	0.8	2.3
T15 (°F)	746	0.7	1.8	864	0.8	2.3
T20 (°F)	760	0.6	1.7	881	0.9	2.6
T30 (°F)	783	0.7	1.9	907	1.0	2.8
T50 (°F)	821	0.7	2.1	942	1.1	3.1
T70 (°F)	859	0.7	2.0	972	1.0	2.9
T80 (°F)	882	0.7	2.0	990	1.0	2.6
T90 (°F)	911	0.6	1.7	1011	0.9	2.4
T95 (°F)	934	0.7	1.8	1027	0.7	2.0
FBP (°F)	997	1.0	2.8	1069	1.9	5.3
Viscosity @ 40°C	41.5	0.4	1.1	117	0.5	1.4
Viscosity @ 100°C	6.3	0.03	0.1	12.2	0.04	0.1
Pour Point	-18.7	0.2	0.6	-14.2	0.2	0.5
Noack Volatility	13.2	0.1	0.3	11.7	0.1	0.4
Aromatics	1.3	0.04	0.01	1.9	0.03	0.08

Table 2. Repeatability results for two standards.

Repeatability

Table 2 compares various properties between two repeatability samples, labeled A and B. The table contains the mean value, standard deviation (StDev), and repeatability coefficient at 95% confidence (RC) for each property. For both samples, the standard deviations and repeatability coefficients are small and within boundaries that indicate the MarqMetrix All-In-One Process Raman Analyzer system can be used for real-time analysis.

Conclusion

In conclusion, the MarqMetrix All-In-One Process Raman Analyzer system, equipped with a MarqMetrix sampling optic, demonstrated high accuracy and reliability in monitoring quality properties of base oils. The strong correlation between measured and predicted values underscores the robustness of the MarqMetrix All-In-One Process Raman Analyzer approach. Overall, the findings highlight the potential of process Raman spectroscopy in general and the MarqMetrix All-In-One Process Raman Analyzer in specific for process monitoring in the refinery operations. This approach not only ensures the consistency and performance of lubricants but also supports predictive maintenance, preventing costly downtime and extending the operational life of industrial equipment.

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