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Use of a digital twin to analyze the effect of graphene as a lubricant additive for diesel engines

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The effect of two graphene additives to engine oil on diesel engine efficiency was studied. The first additive was a commercially available additive based on graphene oxide (GO). The additive was tested on a small automotive diesel engine. The use of the additive concentration recommended by the manufacturer at 3% in the engine oil resulted in a reduction of the specific fuel consumption from 0.2% to 0.7%, depending on the engine operating conditions. The second additive, currently under development, was based on graphene nanoplatelets (GNP). The additive was tested on a medium-sized diesel engine in a truck. The use of the equivalent GNP concentration of 0.1% resulted in a reduction of fuel consumption in the ESC test by 0.4%. Increasing the concentration of this additive to 0.2% GNP did not result in a further reduction in fuel consumption. Because the engine efficiency benefits resulting from the use of improved oils were close to the measurement uncertainties, the applicability of machine learning using engine on-board diagnostics (OBD) readings to analyze the impact of lubricant additives was investigated. The use of Random Forest, machine learning digital twins, was able to reproduce the OBD instantaneous fuel consumption with excellent accuracy. Further analysis with SHAPLEY values helped to identify the more important engine parameters that affected instantaneous fuel consumption.

Key words: *energy efficiency, engine oil, graphene oxide, graphene nanoplatelets, fuel consumption, machine learning, Shapley values (SHAP)*

1. Introduction

Reducing mechanical losses in internal combustion engines is crucial for enhancing efficiency and lowering emissions. Engine oil properties significantly influence these losses [7, 9, 21]. Lower-viscosity oils can decrease hydrodynamic friction, improving fuel economy. However, they may also reduce oil film thickness, potentially increasing wear under certain conditions. To mitigate this, different additives to oil are employed to form protective tribofilms, reducing boundary friction and wear. Studies have shown that combining low-viscosity base oils with effective additives like molybdenum dithiocarbamate (MoDTC) can optimize the balance between friction reduction and component protection, leading to improved engine performance and longevity. Unfortunately, MoDTC, which is a very effective friction modifier, is not used in diesel engines with the Diesel Particulate Filter (DPF) due to its harmful effect on the DPF [8, 22, 23].

Recent advances in nanotechnology have introduced novel lubricant additives, among which graphene-based materials have gained considerable attention due to their outstanding tribological and thermal properties. Graphene oxide (GO) and graphene nanoplatelets (GNP) are among the most commonly investigated forms of graphene for lubricant applications. GO, with its oxygen-containing functional groups, offers good dispersibility in polar and non-polar base oils, enabling the formation of a stable suspension and tribological film. On the other hand, GNPs – few-layer graphene structures with high surface area – demonstrate excellent mechanical strength, load-bearing capacity, and low shear characteristics, making them effective in reducing boundary friction and wear under high-load conditions [1, 3, 12, 15, 17, 18].

Machine learning techniques have shown increased use in helping engine tests. They are able to find complex, nonlinear relationships in data that may be difficult to catch with traditional statistical methods. Machine learning can identify the importance of even those features that have a smaller impact on the output and take them into account in creating predictions [4–6, 10, 16, 19, 24]. The use of digital twins can reduce the number of costly experimental tests and help with the analysis of instantaneous variations. Engine transients, e.g. transients when the engine goes from one operation regime to another, are neglected in stationary tests but may contain relevant information on real driving conditions.

In the current work, two graphene-based lubricant additives were investigated using diesel engine dynamometer tests. Since the expected fuel savings by using improved oils are almost the same as experimental test variability, instantaneous reading of the engine On-Board Diagnostics (OBD) and random Forest machine learning digital twins were used for a more detailed analysis of the effect of the lubricant additives.

2. Tests of a commercially available graphene additive

A commercially available additive with claims of graphene was added to a SAE 5W-30 oil, fully synthetic, Low SAPS. TGA analysis suggests that the additive contains Oxide of Graphene (GO). It was not possible to determine the Graphene concentration in the additive. 3% in volume of additive was added to the engine oil, as recommended by the supplier, for the engine tests. Due to the additive's relatively lower viscosity, oil kinetic viscosities kV40 and kV100 were reduced by about 4%. See details in [11].

An automotive 4-cylinder Diesel engine, 1.25 L, 66 kW, TCDI, Common Rail injection system, air cooling and EGR was tested on a dynamometer with controlled coolant and oil temperatures. The following OBD parameters were recorded at 5 Hz frequency: time, acceleration pedal position, engine rotational speed, total fuel injection, coolant temperature, boost pressure, fuel pressure in the rail, exhaust temperature after DPF, and DPF filling. Potentially interesting parameters, such as injection timing, were not available via OBD on this engine. The dynamometer tests were done at two accelerator pedal positions: 100% and 30%, and engine speeds: 2000 to 4000 rpm. The test sequence was: a) baseline oil, b) addition of 3% VV of the graphene-based additive, as recommended by the additive supplier. Before pouring the additive, the same oil volume was removed from the crankcase to maintain the engine oil volume constant. Maximum engine torque and power increased 0.8% and 0.4% with the oil additive, but as fuel consumption also showed a small increase with the additive, BSFC decreased on average by only 0.2% [11].

Tests for oil without an additive and with the additive were repeated at least 3 times. The repetitions were always done on different days. For simplicity, the dataset was defined as sequential time, including only the OBD acquisitions. Figure 1 shows the test sequence with the reference oil (without an additive). Figure 2 shows the map of engine rotational speed and pedal position covered during the tests.

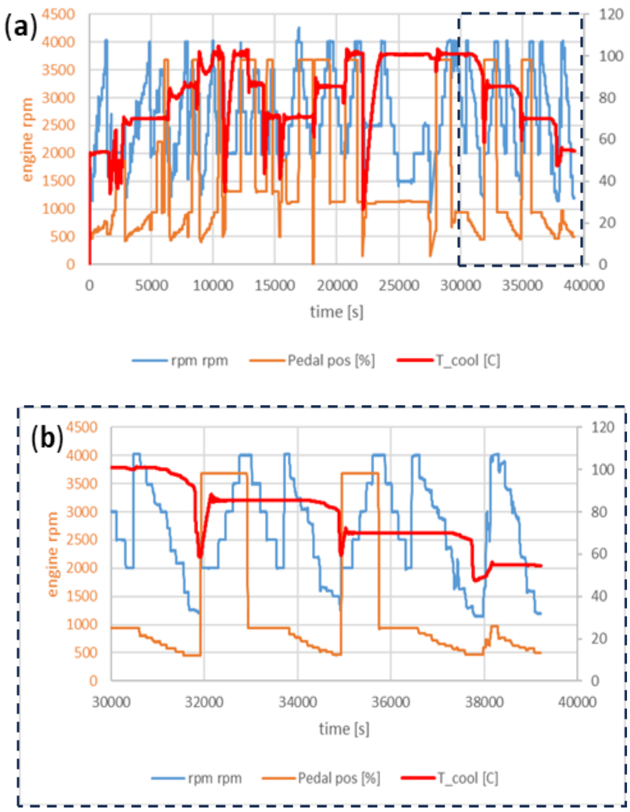

Fig. 1. Test sequence with the reference oil: (a) complete sequence, (b) zoom on the last replications

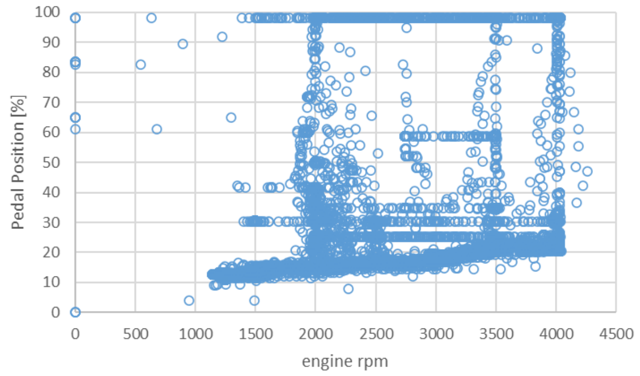

Fig. 2. Map of engine rotational speed and pedal position along the tests with the reference oil

Pearson and Spearman correlations were calculated to select the variables used as input to train the digital twin. Pearson assumes a linear numerical regression, while Spearman is more flexible and calculates the correlation based on the variable ranking. Table 1 shows the Pearson correlation between variables, and Table 2 shows the Pearson and Spearman correlation factors for the instantaneous fuel consumption. Pearson and Spearman's rankings are similar, but notice that some differences exist. See discussion of Shapley values in the MDD case ahead.

Table 1. Pearson correlation coefficients between the variables

	rpm	Pedal Pos	T_cool	P_boost	P rail	Fuel Inj	T_afterDPF	DPF_fill	Fuel Cons.
rpm	1.00	0.25	0.13	0.41	0.64	0.19	0.11	0.25	0.52
Pedal Pos	0.25	1.00	0.08	0.97	0.83	0.99	0.43	0.26	0.92
T_cool	0.13	0.08	1.00	0.11	0.06	0.07	0.15	0.75	0.09
P_boost	0.41	0.97	0.11	1.00	0.84	0.95	0.26	0.34	0.91
P rail	0.64	0.83	0.06	0.84	1.00	0.80	0.35	0.32	0.96
Fuel Inj	0.19	0.99	0.07	0.95	0.80	1.00	0.44	0.26	0.90
T_afterDPF	0.11	0.43	0.15	0.26	0.35	0.44	1.00	0.35	0.44
DPF_fill	0.25	0.26	0.75	0.34	0.32	0.26	0.35	1.00	0.27
Fuel Cons.	0.52	0.92	0.09	0.91	0.96	0.90	0.44	0.27	1.00

Table 2. Pearson and Spearman correlations to the instantaneous fuel consumption

	Pearson	Spearman
rpm	0.52	0.69
Pedal Pos	0.92	0.89
T_cool	0.09	0.19
P_boost	0.91	0.92
P rail	0.96	0.98
Fuel Injection	0.90	0.70
T_afterDPF	0.44	0.19
DPF_filling	0.27	0.37

1.0
0.8
0.6
0.5
0.4
0.2
0.1
0.0

The correlation coefficients show some obvious relations, fuel consumption is directly dependent on fuel injection, boost pressure, etc. To verify the digital twin's capacity to make predictions with as few parameters as possible, the following parameters were selected to predict the instantaneous fuel injection:

- inputs: engine rotational speed, pedal position, cooling temperature
- output, "target" in the machine learning jargon: fuel injection or fuel consumption, the latter calculated from the OBD fuel injection and engine rotational speed.

The machine learning digital twin is created ("trained" in the AI jargon), having variables for input and, in our case, one for output to be predicted (Fig. 3–5).

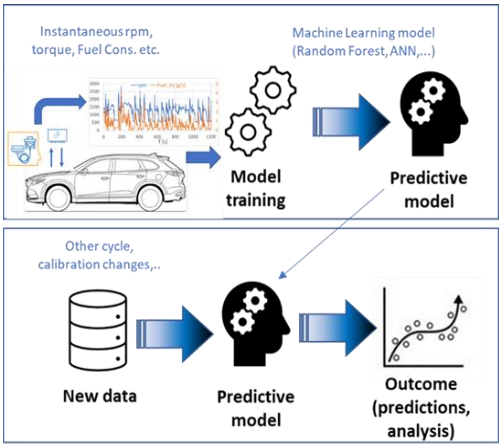

Fig. 3. Scheme of the machine learning approach used in this work (reproduced from [19])

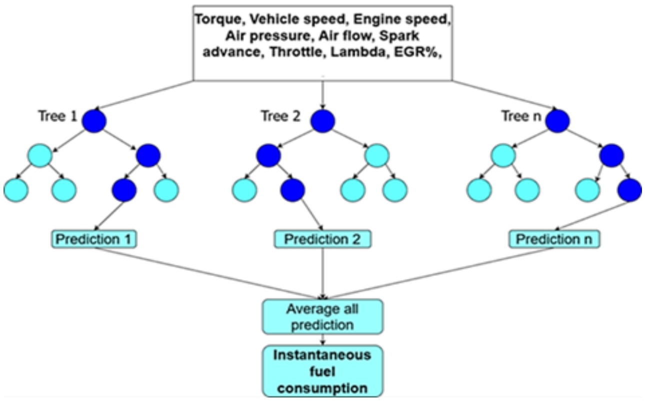

Fig. 4. Scheme of the machine learning Random Forest model (reproduced from [19])

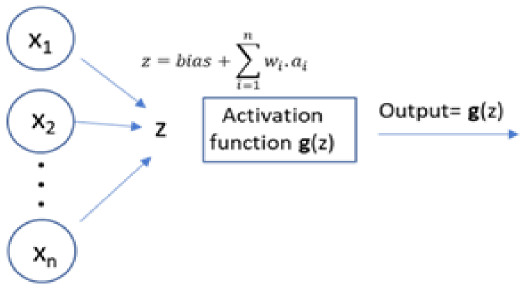

Fig. 5. Scheme of the Random Forest model (reproduced from [19])

In all replications, the model correlation between the real ECU instantaneous fuel injection and the model was very good, with a coefficient of correlation R^2 of almost 1.0 and an accumulated error smaller than 0.1%. See two examples in Fig. 6 and Fig. 7. Such good correlation was already verified in the author's previous publications, even for transient emission and RDE cycles [14]. More robust validation is whether the model trained on a given day can predict the test on another day, which was also obtained with the developed digital twin. Figure 7 shows that the model prediction for the 2024Feb06 test using the model trained with the baseline 2023 dataset showed an almost perfect correlation, R^2: 0.9994, and the accumulated error on accumulated fuel injected along the replication was lower than 0.1%. The time frames in Fig. 6–9 refer to the respective test replication (06_02 and 07_02). They are part of the complete test sequence shown in Fig. 1, but with time starting at the start of the respective replication.

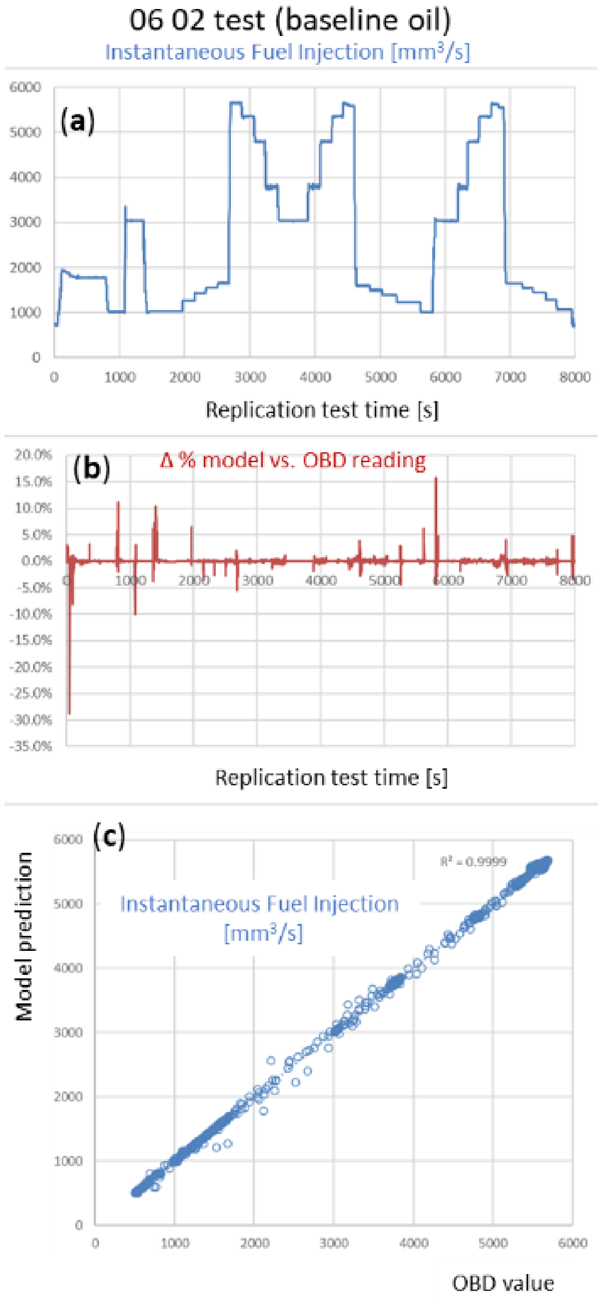

Fig. 6. Digital twin predictions for the reference test

As already mentioned, using the dynamometer stand measurements, BSFC reduction was almost within the experimental uncertainties [11]. To investigate if the use of digital twins could provide a more resolute comparison, the following method was carried out:

– instantaneous fuel consumption was calculated using the fuel injection and engine rotational speed

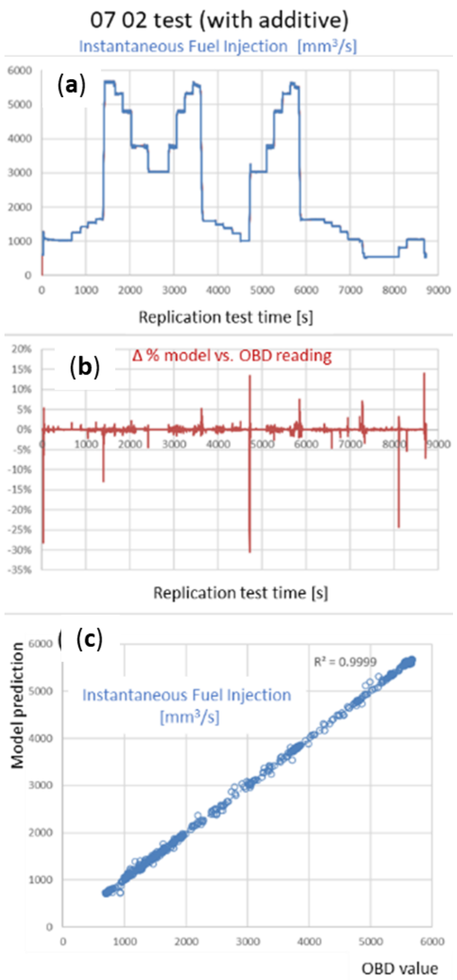

Fig. 7. Digital twin predictions for test with 3% additive

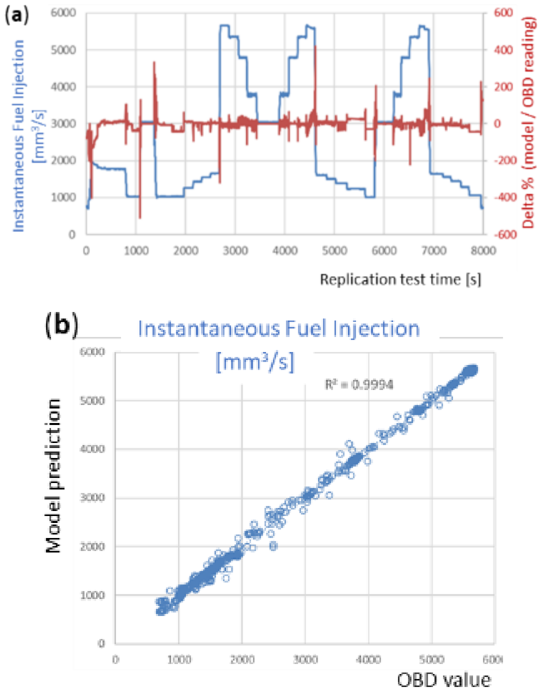

Fig. 8. Prediction for the 06Feb2024 replication with the model trained with Dec2023 replications

– 2 digital twins were trained for tests done on consecutive days, one with the baseline oil, and the other with the addition of the 3% V/V graphene additive. Both models were able to fully reproduce the respective datasets, as discussed before
– then, the model trained with the baseline oil was used to predict the test with the graphene additive and vice versa.

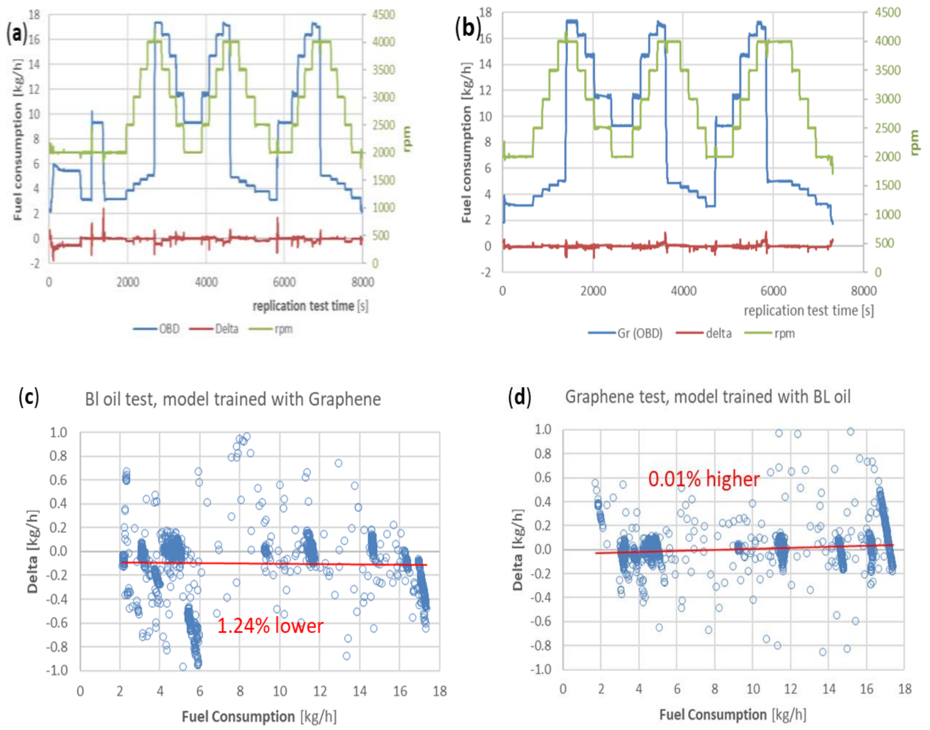

Fig. 9. Tentative to use the digital twins to predict the influence of graphene on instantaneous fuel consumption: (a) and (c) reference oil test, model trained with graphene; (b) and (d) test with graphene, model trained with the baseline oil

The expectation was that the model trained with graphene would reduce the fuel consumption when applied to the baseline oil, and the opposite when the baseline oil model was applied to the test with graphene. However, the results were inconclusive. While the model trained with graphene reduced 1.24% the fuel consumption of the baseline test, the use of the baseline oil model showed almost no change when applied to the test with graphene. See Fig. 9.

3. Tests of a GPN-based additive

After testing the GO additive on the small diesel engine, the project moved to the use of an in-house graphene-developed additive based on graphene nanoplatelets (GNP) with a higher graphene concentration. Table 3 and Fig. 10 show the GNP main characteristics. See details in [20]. The higher graphene concentration allowed a reduction in the additive volume, leading to a lower impact on the kinematic viscosity of less than 1%.

Table 3. GNP characterisation

Characteristic	Unit	Mean	Q90
Number of layers – <N>2D (nm)	–	9	11
Surface density of point defects – nD	10^{10} cm^{-2}	2.8	4.3
Lateral size – L_a	nm	71.1	99.4
D to G peak intensity ratio (I_D/I_G)	–	0.28	0.44

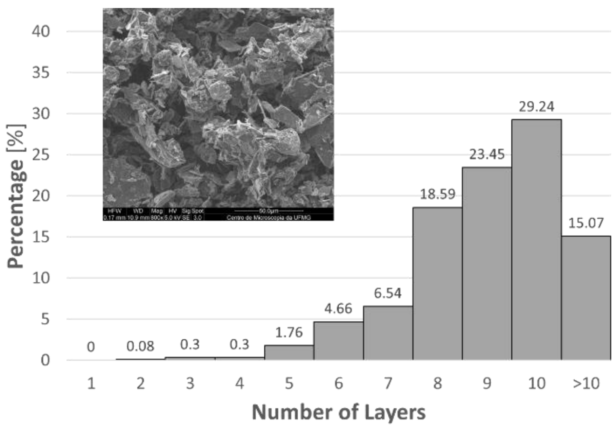

Fig. 10. GNP number of layers, adapted from [20]

A Medium-Duty Diesel (MDD) engine of 4.8 L, 4-cyl., 136 kW and 700 Nm was used in the tests. Both the DPF sensor and the coasting strategies were turned off during the tests. The dynamometer tests were carried out in the following sequence: a) baseline oil, b) addition of the equivalent of 0.1% graphene, c) another 0.1%, reaching a total of 0.2% of graphene. The test cycle followed the European Stationary Cycle (ESC) – see Fig. 11. Four other operation regimes, at engine rotational speed of maximum power and 25, 50, 75 and 100% of load were added to the test program for completeness.

On the combined ESC values, 0.4% and 0.3% fuel saving were observed with 0.1% and 0.2% graphene additives, respectively – see [11]. The possibilities of using AI in the results obtained in MDD tests were initially investigated in [14]. Digital twins were able to reproduce the OBD values accurately. In the current work, an improved digital twin and the calculation of SHAP values were used to understand better the potential and limitations of using AI on fuel consumption tests.

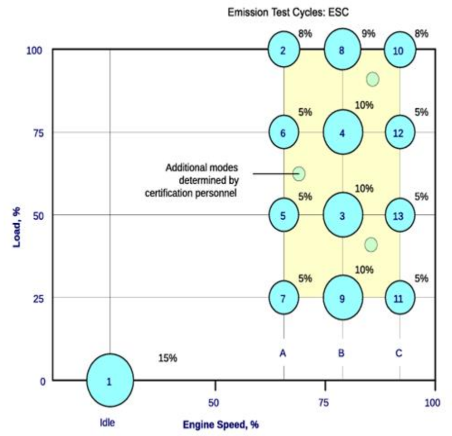

Fig. 11. ESC cycle

On the ESC cycle, the engine must be operated for 2 minutes at each regime point. At each point, the first 20 seconds are neglected to allow engine stabilization. But even after stabilization, it is not uncommon that some engine parameters present instantaneous variations. For example, Fig. 12 shows turbo pressure variations, which may affect instantaneous power, fuel consumption etc. Figure 13 shows in more detail step 11, neglecting the first 20 seconds as defined in the ESC procedure. The step average is 1791 hPa and 7.0 kg/h, respectively, for turbo pressure and fuel consumption. However, it can be noted that there is lower fuel consumption when the P_turbo is higher than the average and higher fuel consumption when the P_turbo is lower than the average. Such a correlation, although small, is not considered if only the average values are considered.

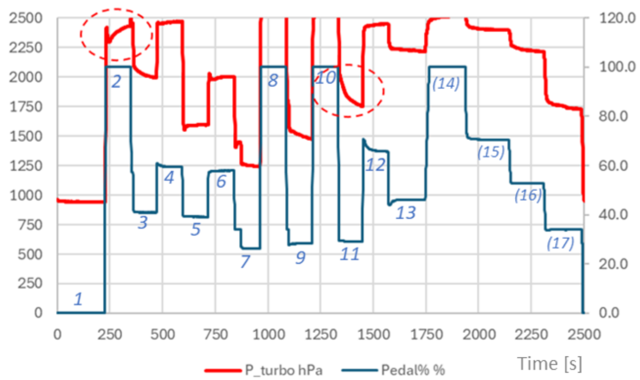

Fig. 12. OBD turbo pressure and pedal position along a tests sequence; notice some instantaneous variations even on stationary conditions

Table 4 shows the four higher Pearson correlation coefficients used as input to train the digital twin. These chosen parameters are engine speed, coolant temperature, turbocharger pressure and calculated torque, so-called rpm, Tcool, P_turbo and CalcTorque, respectively. No significant difference was found in the correlation coefficients between the baseline oil and the ones with graphene additives.

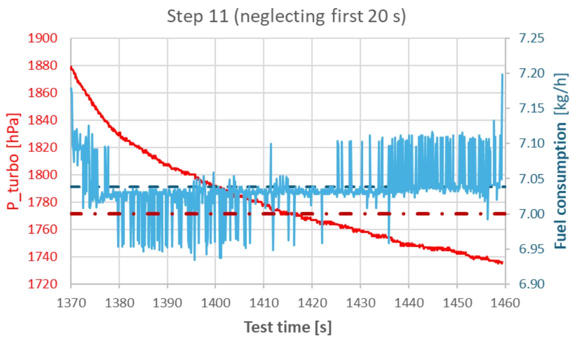

Fig. 13. Turbo pressure and fuel consumption for step 11 – see Fig. 12

Some of the parameters may indeed be an indirect consequence of fuel consumption. For the carried-out tests, with the engine already hot, the engine cooling temperature was probably affected by the torque (and not vice versa). The higher torques caused, of course, higher fuel consumption. See discussion ahead.

The developed digital twins were able not only to reproduce the test used for training accurately but also to predict the instantaneous fuel consumption of a different replication – see Fig. 14–18.

Table 4. Pearson correlation coefficients for the four parameters used to train the digital twin

	baseline oil							+ 0.1% graphene									+ 0.2% graphene					
	BL_18	BL_19	BL_20	BL_22	BL_25	BL_26		0.1_29	0.1_30	0.1_32	0.1_33	0.1_35	0.1_36	0.1_38	0.1_39		0.2_41	0.2_42	0.2_44	0.2_45	0.2_47	0.2_48
rpm	0.58	0.56	0.54	0.56	0.53	0.51		0.57	0.52	0.51	0.51	0.53	0.54	0.54	0.48		0.53	0.54	0.55	0.53	0.56	0.53
Tcool	0.67	0.64	0.63	0.61	0.60	0.59		0.62	0.59	0.58	0.58	0.57	0.58	0.61	0.59		0.57	0.59	0.60	0.60	0.61	0.56
P_turbo	0.93	0.93	0.93	0.93	0.92	0.92		0.93	0.93	0.93	0.93	0.93	0.93	0.93	0.93		0.93	0.93	0.93	0.93	0.93	0.93
CalcTorque	0.92	0.92	0.92	0.92	0.92	0.92		0.93	0.92	0.93	0.92	0.92	0.92	0.92	0.92		0.92	0.92	0.92	0.92	0.92	0.92

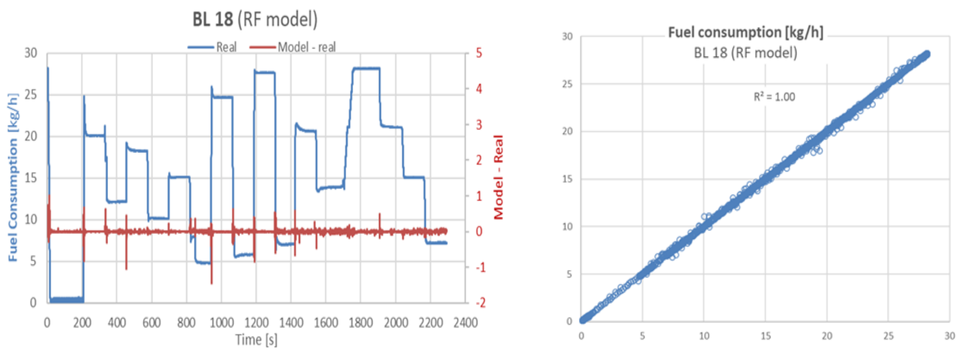

Fig. 14. RF digital twin for the baseline oil replication #18

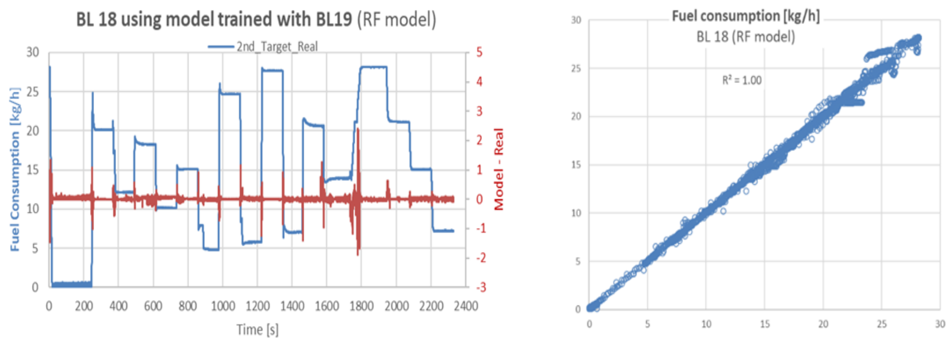

Fig. 15. RF digital twin, trained with replication BL #19, for the BL #18

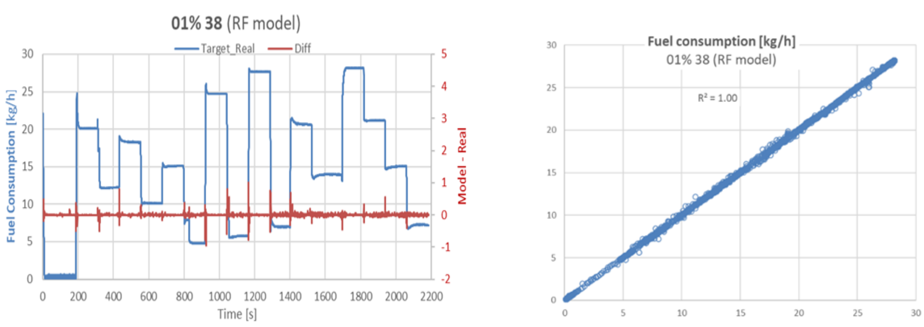

Fig. 16. RF digital twin trained with replication #38 with 0.1% GNP

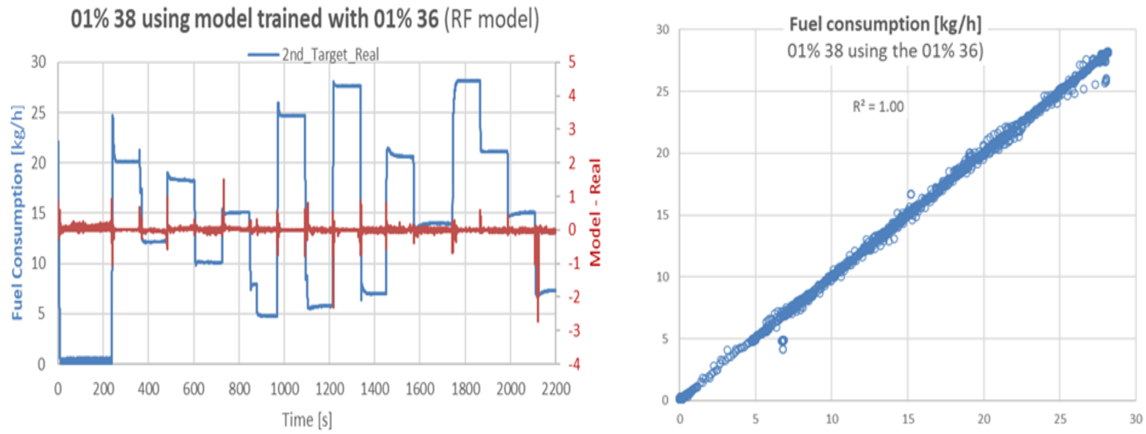

Fig. 17. RF digital twin, trained with replication 01% #36, for the 0.1% #38

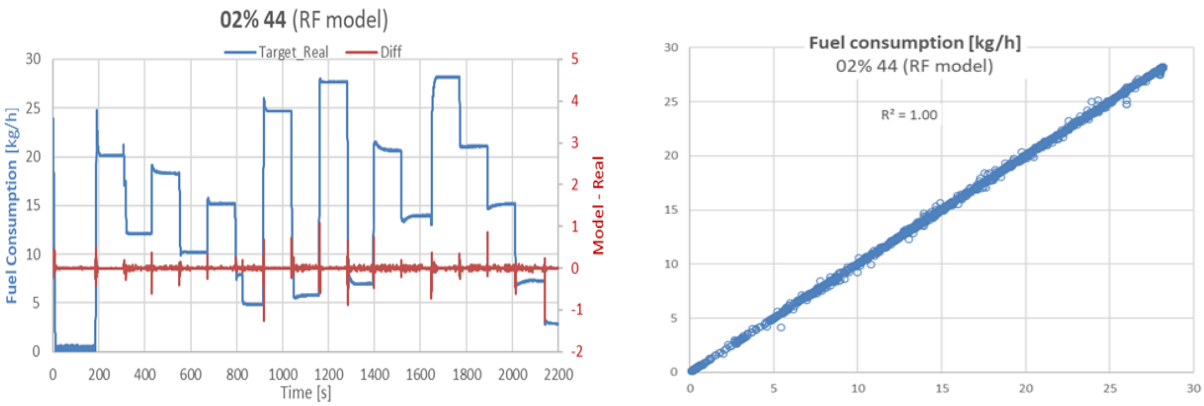

Fig. 18. RF digital twin, trained with replication 0.2% #44

4. Use of SHAP values to analyze the digital twin model

The correlation factor calculations were carried out in the datasets and do not necessarily reflect the impact on the model output. SHAP (SHapley Additive exPlanations) is a method used to explain how machine learning models make predictions. It is based on ideas from cooperative game theory, especially Shapley values, which fairly measure each player's contribution in a group. In machine learning, SHAP looks at how important each feature (or input) is to a specific prediction. It shows how much each feature pushes the prediction higher or lower by comparing the result with and without that feature [2, 13].

SHAP helps explain both individual predictions (local explanations) and overall model behavior (global explanations). This is especially useful for complex models like neural networks or ensemble methods, where understanding how they work is often difficult. Because SHAP adds up all feature contributions to match the model's output, it makes model decisions easier to trust and understand [2, 13].

Figure 19 presents a SHAP summary plot, which illustrates the impact of each feature on the model output across the entire dataset. Each point in the plot represents a SHAP value for an individual prediction, showing how much that feature contributed to increasing or decreasing the prediction.

The features are ranked vertically by their overall importance (mean absolute SHAP value), with the most influential features at the top. In this case, Pedal%, P_turbo, and rpm are the most impactful features in predicting the model output. The color of each point represents the original value of the feature for that observation, ranging from low (blue) to high (red). For example, for Pedal%, high feature values (in red) are generally associated with a strong positive impact on the model output, whereas lower values (in blue) tend to have a negative contribution.

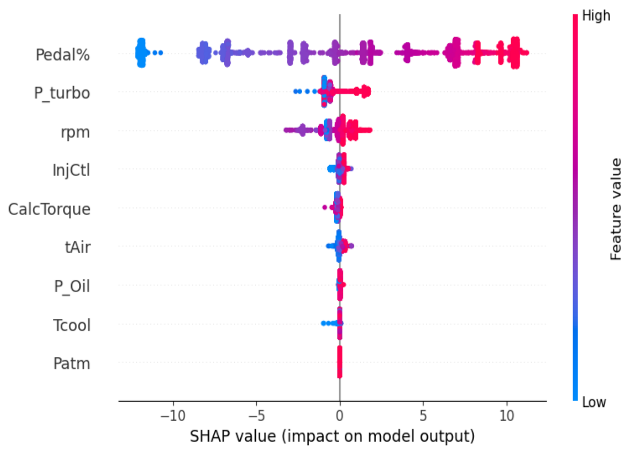

Fig. 19. SHAP Summary Plot for Feature Impact and Direction

The horizontal dispersion of points for each feature reflects the range of SHAP values and thus the variability in that feature's influence. Features like Pedal% and P_turbo show wide distributions, indicating that their impact on predictions varies significantly across the dataset. This visualization helps to understand not only which features are most important but also how their values influence the model's behavior, enabling better transparency and interpretability of the predictions.

Figure 20 shows the SHAP bar plot for the baseline test. The plot summarises the average impact of each feature on the model's predictions, measured by the mean absolute SHAP value. Pearson and Spearman correlations are also shown for comparison. The Pedal% is the most influential feature, followed by P_turbo and rpm, indicating their strong contribution to model output. Other features like InjCtl, CalcTorque, and tAir have a moderate influence, while P_Oil, Tcool, and Patm contribute minimally. This plot provides a clear overview of the importance of global features, supporting model interpretation and validation.

Notice that several parameters with high Pearson and Spearman correlation have little or no impact on the digital twin. A remarkable example is the CalcTorque with correlation factors close to 0.9, but very little effect on the model output.

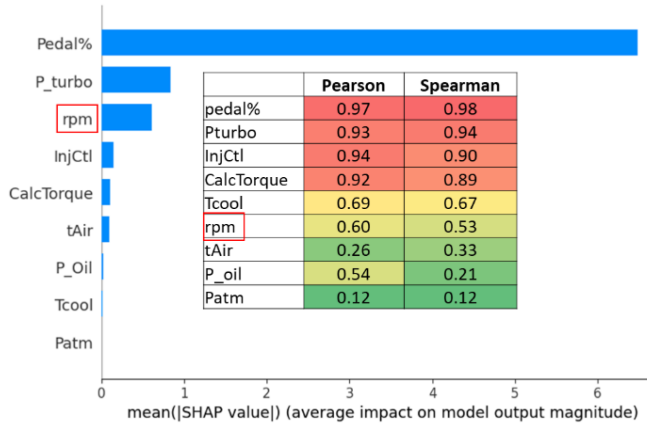

Fig. 20. Global Feature Importance Based on SHAP Values

5. Discussion and conclusions

Even under stationary conditions, normal variations in engine combustion cause instantaneous changes in engine parameters and outputs, such as power and fuel consumption. Such instantaneous variations contribute to experimental errors and may contain some relevant information that is lost when only the average values are considered. The use of instantaneous readings, either by dynamometer measurement equipment or by OBD readings, can help a more resolute analysis.

The use of machine learning models using instantaneous readings from the engine OBD showed promising results. The models are able not only to reproduce the test replication used for training but also other replications. The use of the OBD reading, digital twin and SHAP values also allowed a better assessment of the parameters impacting the engine efficiency that would be difficult to assess using conventional test methods. After the SHAP analysis mentioned before, a dataset combining three replications of each variant, Baseline, 0.1 and 0.2% GNP, was created by merging the individual tests. The created dataset had 208181 instantaneous OBD readings. The digital twin used as input only the Pedal%, rpm and the GNP concentration. The digital twin accuracy was excellent, R^2 = 1.00, Mean Squared Error, MSE, 1.6E–3 and the accumulated fuel consumption error was lower than 0.01% (Fig. 23 and Fig. 24).

The impact of the GNP additive was very low in the carried, stationary tests. Indeed, it is known that the impact of lubricant formulation is low on diesel engines operating at higher loads. The same GNP additive, L66_2, was tested with success on SI vehicles under the FTP75 cycle [20]. Improved additives and truck transient tests are ongoing and will be covered in future publications.

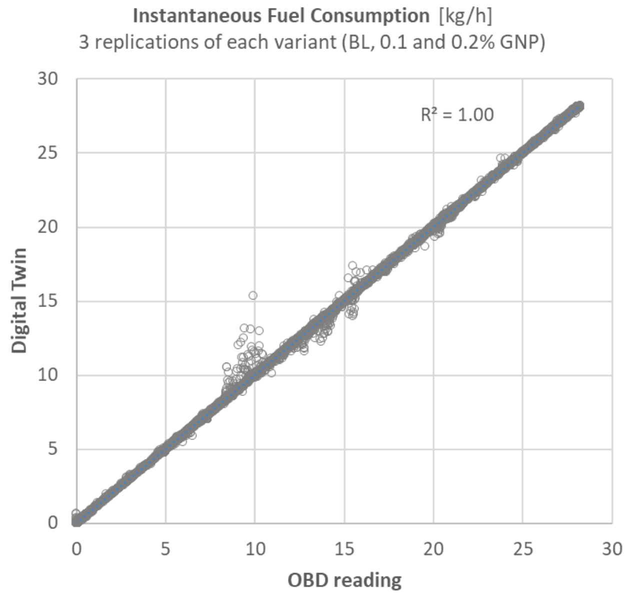

Fig. 21. Digital twin of three replications of each lubricant variant, trained only with Pedal%, rpm and GNP concentration as input

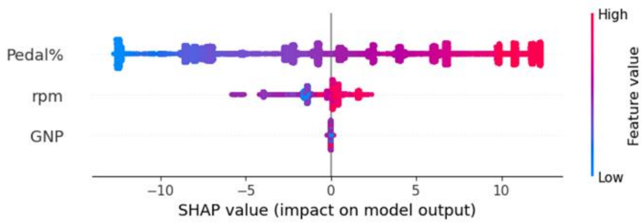

Fig. 22. SHAP summary for the digital twin with three replications of each lubricant variant

The main conclusions from the research conducted are as follows:

- the use of Random Forest, machine learning digital twins, allowed for the reproduction of the actual values of fuel consumption with very good accuracy
- use of Pearson and Spearman correlations to select the model input parameters can lead to the inclusion of unnecessary parameters, which not only increases computer resources but can also lead to erroneous analysis

– use of SHAP values can better indicate the parameters influencing the output and a better understanding of the physical system and the digital twin model, somehow "opening" the AI black box, which will be explored in more complex and transient tests.

Nomenclature

AI artificial intelligence
BL baseline
DPF diesel particulate filter
ESC european stationary cycle
GNP graphene nanoplatelets
GO graphene oxide
MDD medium-duty diesel
MoDTC molybdenum dithiocarbamate
OBD on-board diagnostics
RDE real driving emissions
SAPS sulphated ash, phosphorous, and sulphur
SHAP Shapley additive explanations
TCDI turbo common rail direct injection
TGA thermogravimetric analysis

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