Prediction of Bitumen Ageing States Using the Kernel Ridge Regression Model

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ABSTRACT: The study presents the first results of a supervised machine learning model used to predict the complex modulus of both neat and aged binders recovered from asphalt concrete. Trained on data combining complex modulus measurements and chemical properties, the model captures the intricate relationships between bitumen composition and mechanical behaviour. The model successfully predicts both known and unknown ageing states.

1 INTRODUCTION

The binder of hot mix asphalt undergoes two successive chemical ageing phases: rapid ageing during production and construction (short term) and slow ageing over the pavement's lifespan (long term). Oxidation is the main cause of bitumen ageing (HUNTER et al., 2015, p. 75 and 575). At the coating stage, oxidation is intense due to the high temperatures and air exposure, whereas in service, bitumen oxidises slowly in the presence of temperature cycles and oxygen from atmospheric air.

To replicate these ageing phases, accelerated artificial ageing processes have been developed in laboratories. These processes have shown that bitumen ageing alters both its chemical composition and rheological behaviour over time. Internationally recognised physico-chemical indicators are used to assess the brittleness of binders or mixtures with respect to the cracking risk (KHANDAL, 1977, ROWE, 2011, SIROMA et al., 2024). However, to date, there is no established model linking rheological changes observed at different ageing stages and across material scales (binder, mastic, asphalt mix).

In parallel, the use of Artificial Intelligence (AI) is expanding in the field of pavement materials. Supervised learning, a subset of machine learning, involves learning a predictive function from labelled examples (ZHOU, 2021). Its application could help establish transition laws between ageing states, linking binder rheology to that of the asphalt mix.

This article presents a preliminary study that explores a supervised learning approach to predict bitumen rheology at a given ageing state based on prior states. Rheological properties, serving as physical markers of ageing, are characterised here through complex modulus tests. Traditionally, these data are modelled with rheological equations, while the effects of temperature, loading amplitude, and thixotropy are approximated through translation principles (COULON et al., 2021). However, ageing modifies the shape of complex modulus curves, requiring constant recalibration of these equations. A simple translation principle cannot be applied to model ageing, which has led to the adoption of a supervised approach to bypass this limitation.

Each ageing state is further associated with chemical markers, including SARA fractions (saturates, aromatics, resins, asphaltenes) and carbonyl and sulfinyl indices, which reflect oxidation levels. The model aims to identify the relationships between the chemical composition of bitumen and its rheological properties.

The article is structured as follows. First, the bitumen from the MoveDVDC project and its associated physical and chemical data are introduced. Next, the Kernel Ridge Regression model, a supervised learning model, is adapted for this study. Finally, the results are analysed and discussed.

2 MATERIALS

The French ANR MoveDVDC project (2018-2023) has generated a substantial database of asphalt mixtures and bituminous binders extracted *in situ* or produced in a laboratory using ageing protocols (Siroma, 2022). This paper focuses on the physico-chemical data for eight ageing states of the bitumen binder A3550_C.

The bitumen in question is extracted from a GB3 (a French asphalt concrete meaning Grave-Bitume class 3) prepared and aged in a laboratory. This asphalt mix is made of 0/14 mm limestone aggregates and a pure bitumen of penetration grade 35/50 dosed at 4.5% of the mass of dry aggregates. The aggregates and the bitumen were initially heated overnight to 165°C and 110°C respectively. The temperature of the bitumen was then increased to match that of the aggregates for approximately two hours. Finally, the two components were mixed using a mixer for about three minutes until the aggregates were completely coated with bitumen. The mixture has a true density of 2509 kg/m^3.

After the mixing stage, an ageing protocol proposed by La Roche et al. (2009) was applied to the expanded asphalt of GB3. To simulate short-term ageing, the asphalt mixture was first spread uniformly in metal trays to a thickness of around 5 to 6 cm. The trays were then placed in a forced-draught oven at 135°C for 4 hours. The mix was stirred for one minute every hour. To reproduce long-term ageing, the asphalt mix was then conditioned at 85°C for 2, 5, 7, 9 and 20 days. After each ageing stage, the bitumen was extracted to study its characteristics.

To define physical markers, complex modulus tests were carried out on the bitumen using a Dynamic Mechanical Analysis (DMA) rheometer. The device was placed inside a thermal chamber. At low temperatures (≤ 20°C), the test was carried out in direct tension-compression on a cylindrical specimen. At high temperatures (> 20°C), the test was carried out using annular shear on a hollow cylindrical specimen. Conversion from norm $|G^*|$ to $|E^*|$ was performed considering a constant Poisson's ratio of 0.50. The tests were conducted by strain amplitude control (close to 50 μm/m) with frequency sweeps (from 1 to 80 Hz) at different temperatures (from -15 to 70 °C). A minimum of two repetitions were performed for each sample, provided that the variations in $|E^*|$ and φ_{E^*} were less than 15% and 5% respectively. The data are presented in Figure 1 using the stiffness $\mathfrak{R}_E$ and viscosity $\mathfrak{I}_\eta$ components (Coulon et al. 2021) such as:

$$\sigma(t,T,\omega) = \mathfrak{R}_E(T,\omega)\varepsilon(t,\omega) + \mathfrak{I}_\eta(T,\omega)\dot{\varepsilon}(t,\omega) \quad (1)$$

Where $\sigma(t)$ and $\varepsilon(t)$ are respectively the stresses and strains of the DMA test. The temperature T and pulsation ω effects can be associated into a single parameter, the reduced pulsation ω_{R-T}, according to the Time-Temperature Superposition Principle (TTSP). Table 1 gives the coefficients $C_{1,aT}$ and $C_{2,aT}$ of the Williams-Landel-Ferry (WLF) law at the reference temperature of 0°C.

Two other analyses were carried out to identify chemical markers. First, Fourier Transform InfraRed spectroscopy (FTIR) was used to monitor the oxidation of the bitumen by calculating the carbonyl I_{CO} and sulfinyl I_{SO} indices, as indicated by LPC test method No. 69 (LCPC 2010). A minimum of five samples were studied for each ageing condition. Second, based on its polarity, bitumen can be separated into four fractions called SARA. The High Performance Thin-Layer Chromatography (HPTLC) was carried out. Table 1 shows the average of these results.

3 APPLICATION OF SUPERVISED MACHINE LEARNING

The primary objective of this section is to train the AI model on the provided experimental data. The ageing of A3550_C bitumen is categorised into eight distinct states. The rheology of each state is represented by the pair of stiffness $\mathfrak{R}_E(\omega_{R-T})$ and reduced viscosity $\mathfrak{I}_{\eta,R-T}(\omega_{R-T})$ at 0°C. To quantify the ageing level, these pairs are associated with a sextuplet of chemical markers, consisting of the I_{CO} and I_{SO} indices along with the four SARA fractions. Once trained, the model is expected to reproduce known ageing states and predict new ones.

Table 1. WLF coefficients at a reference temperature of 0°C, CO and SO indices, and SARA fractions of the bitumen A3550_C at different ageing levels (‘h’ for hours and ‘d’ for days).

Ageing levels	**TTSP $C_{1,aT}$ [-]**	**TTSP $C_{2,aT}$ [°C]**	**FTIR CO [-]**	**FTIR SO [-]**	**SARA Saturate [%]**	**SARA Aromatic [%]**	**SARA Resin [%]**	**SARA Asphaltene [%]**
After heating	21.6	132.1	-0.37	5.06	16.10	46.95	22.30	14.60
After mixing	18.0	113.3	1.28	8.07	16.05	46.50	23.70	13.65
4h	23.5	146.3	2.74	10.26	15.50	45.65	26.90	11.90
4h+2d	23.4	145.1	4.36	12.63	16.30	43.00	29.10	11.60
4h+5d	24.6	150.4	4.53	13.70	15.25	43.60	29.50	11.60
4h+7d	26.6	162.6	5.56	15.42	14.70	44.15	29.70	11.50
4h+9d	24.9	153.4	6.15	14.96	14.15	44.15	31.35	10.40
4h+20d	27.0	163.3	7.82	16.03	14.65	41.20	34.50	9.60

3.1 *Model used*

For this study, the Kernel Ridge Regression (KRR) algorithm was employed with the Radial Basis Function (RBF) kernel (Schölkopf & Smola, 2002). This method is well-suited for solving regression problems involving complex and non-linear relationships between input data X and output data Y, while incorporating effective regularisation to mitigate overfitting (e.g., avoiding an overly complex model that captures noise instead of meaningful trends).

The KRR-RBF algorithm is governed by two key hyperparameters that affect its performance:

- The regularisation parameter λ controls the influence of isolated or atypical data points. A higher λ reduces sensitivity to noise and specific details.
- The γ parameter of the RBF kernel determines the range of influence a data point has on its neighbors in kernel space. A smaller γ results in a smoother model that captures broader trends while ignoring finer local variations.
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The program was developed in Python.

3.2 *Training*

The model incorporates input data, consisting of reduced pulsations and chemical markers for all ageing states. The output data consists of stiffness-viscosity pairs. Since the pulsation, stiffness, and viscosity values span several orders of magnitude, it is crucial to linearise these values by using their logarithms. This step ensures the model avoids producing outliers.

There are several options for selecting the chemical markers. If the model is trained on all six markers, six input values must be provided. However, this approach requires understanding the relationships between these markers to make predictions with hypothetical values. Among the chemical markers, some are more sensitive to ageing than others, such as the I_{CO} and I_{SO} indices and the resin fraction. This study focuses on resins as the primary input.

The other chemical markers could be included as output variables, but in this case, the AI would identify relationships between pulsations and these markers. While this approach causes only slight fluctuations in the markers, they are expected to remain constant with respect to pulsation.

To optimise the hyperparameters, the GridSearchCV algorithm is employed. This method systematically tests all possible combinations of the values provided in the lists for λ and γ (e.g., [10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1, 10]). Based on this process, the optimal values identified for λ and γ are 0.0001 and 0.001, respectively.

3.3 *Model testing and analysis*

To test the model, input data is provided consisting of the range of pulsations and only the resin fraction of bitumen. The model then predicts the corresponding stiffness-viscosity pairs. Figure 1 displays the model's predictions for resin fractions of 18%, 28%, and 38%.

Overall, the results obtained are very satisfactory and encouraging. Although the input pulsations differ between ageing states due to the application of the TTSP, the model still successfully identifies the relationships between the data. This indicates that a

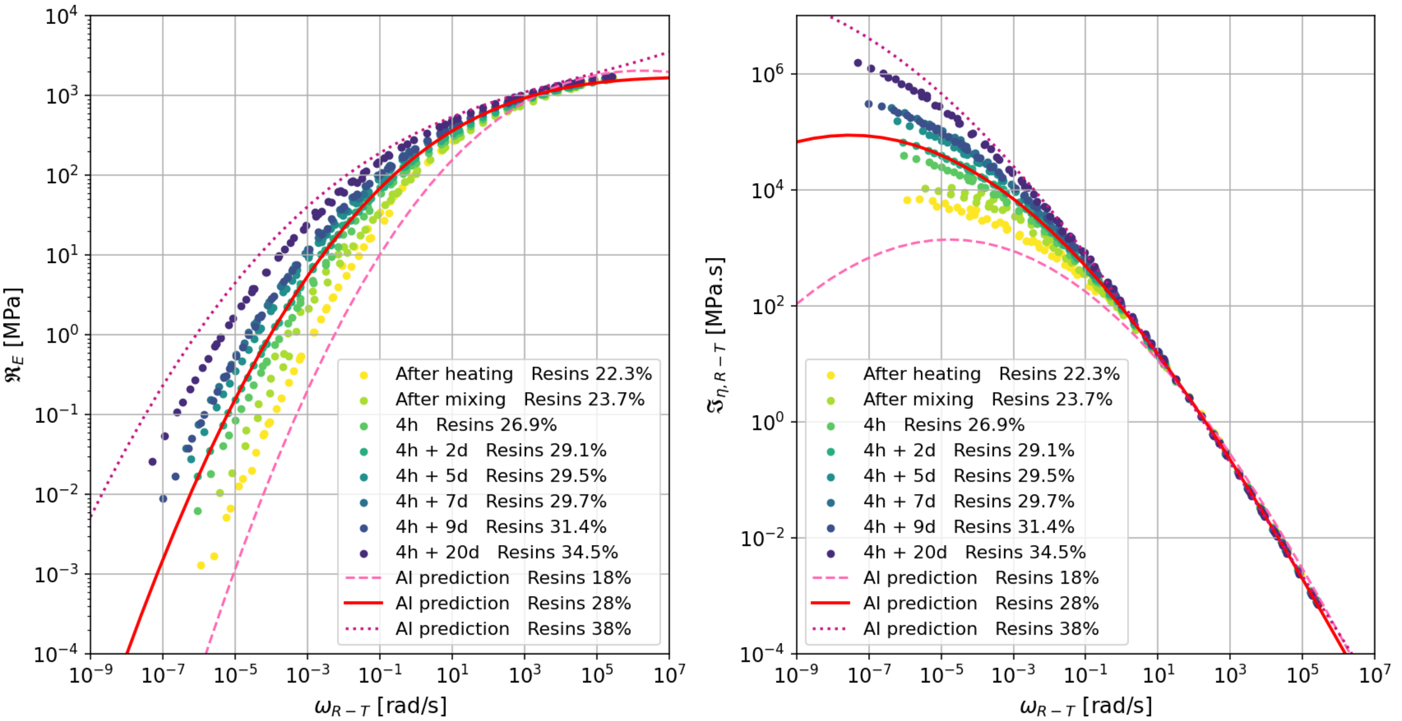

Figure 1. Effect of chemical ageing on the rheology of bitumen A3550_C.
Representation of stiffness $\Re_E$ (left) and reduced viscosity $\Im_{\eta,R-T}$ (right) as a function of reduced pulsation ω_{R-T} at the reference temperature of 0°C. The points represent experimental data, while the lines represent AI predictions for different resin contents.

common pulsation scale across different ageing states is not necessary.

For a given ageing state, the stiffness and viscosity evolve as expected. However, the model does not fully capture the trend where $\Re_E$ and $\Im_\eta$ approach plateaus at high and low pulsations, respectively. Using the RBF kernel, the fitted function is represented as a sum of “bells” centred around each training point. Thus, testing other types of kernels, such as the “sigmoid” kernel, could provide further insights.

The model appears to capture the transition between ageing states well. For the 28% resin fraction prediction, the curve aligns with the ‘4h + 2d’ ageing, corresponding to 29.1%. The 1% difference can be attributed to the model's adaptation to certain inconsistencies in the experimental data, such as the overlap between the ‘4h + 7d’ and ‘4h + 9d’ ageing states, which are similar in terms of stiffness and viscosity despite differing by 2% in fraction. The predictions for 18% and 38% resin fractions are consistent, but predictions tend to become less reliable as we move further from the training data zone.

4 CONCLUSION

The study demonstrated the predictive capability of the Kernel Ridge Regression model when applied to aged bituminous binders. The model successfully captures complex relationships between bitumen chemistry and its mechanical properties and is capable of accurately extrapolating these relationships beyond the training data.

However, while the experimental data used may be considered abundant for the pavement domain, they are limited to a single bitumen type. To enhance the model's robustness, future work should extend the study to include other bituminous materials from the MoveDVDC project and potentially expand it to materials from the ViscoMatData database at Gustave Eiffel University.

Other machine learning models, such as Support Vector Regression (SVR), Random Forest, and Gradient Boosting, should also be tested. Artificial Neural Network (ANN) models could be explored with a larger dataset.

This study also presents several perspectives:

- If we assume that there is a unique SARA fraction decomposition for each stiffness-viscosity curve, it follows that by knowing the chemistry of the bitumen, we might predict its rheology, and *vice versa*.
- The study could serve as a foundation for investigating the transition from bitumen rheology to asphalt rheology.
- In the more distant future, one might envision that, by knowing the age of a pavement and its initial rheology, we might predict whether maintenance would be necessary.

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