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Machine-Learning Prediction of Marshall Mix-Design Properties and Mechanical Characterization of DCR-Treated Asphaltic Concrete

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ABSTRACT: Marshall mix design remains the dominant empirical framework for proportioning hot-mix asphalt, and coconut-derived by-products such as Desiccated Coconut Residue (DCR) have attracted interest as sustainable bitumen modifiers. Determining the optimum bitumen content (OBC) and characterizing mechanical performance is laboratory-intensive, which motivates data-driven prediction. This study evaluated whether regression models can predict six Marshall responses for DCR-modified asphalt concrete and characterized the mechanical performance of the modified mixtures at their respective OBC. Thirty averaged Marshall records covering bitumen contents of 4–6 %, two gradations (AC14, AC20), and three treatments (Control, untreated DCR, treated DCR) were modeled using eight algorithms and a quadratic response-surface baseline. Models were assessed by pooled out-of-fold prediction under random K-fold, leave-one-mixture-out, and leave-one-bitumen-level-out validation. For the AC14 mixtures, OBC values were 5.30% (Control), 4.95% (untreated), and 5.10% (treated); resilient modulus, indirect tensile strength (ITS), tensile strength ratio (TSR), and dynamic creep were measured for each mixture prepared at its own OBC. Pooled out-of-fold R^2 reached 0.89 for voids filled with bitumen, 0.88 for air voids, 0.83 for bulk density, 0.81 for voids in mineral aggregate, 0.53 for flow, and 0.49 for stability. The quadratic response surface matched or exceeded the machine-learning models on four of six responses. Under leave-one-mixture-out validation, R^2 became negative for most responses, whereas leave-one-bitumen-level-out validation retained R^2 of 0.47–0.91. The models are therefore interpolation tools within the tested design space rather than general predictors. The untreated mixture required the lowest binder content, and the treated mixture recorded the highest dry ITS (1,148.7 kPa) and TSR (50.3%), although all mixtures fell below common TSR acceptance limits despite the hydrated-lime filler.

ABSTRAK: Reka bentuk campuran Marshall, kekal sebagai kerangka empirik utama bagi menentukan kadar campuran asfalt panas, dan hasil sampingan berasaskan kelapa seperti Sisa Kelapa Kering (DCR) telah menarik minat pengubah suai bitumen yang mampan. Penentuan kandungan bitumen optimum (OBC) dan pencirian prestasi mekanikal memerlukan kerja makmal yang intensif, sekaligus mendorong penggunaan ramalan berasaskan data. Kajian ini menilai sama ada model regresi mampu meramal enam tindak balas Marshall bagi konkrit asfalt terubah suai DCR, serta mencirikan prestasi mekanikal campuran tersebut pada OBC masing-masing. Sebanyak 30 rekod Marshall purata merangkumi kandungan bitumen 4–6 %, dua gradasi (AC14, AC20) dan tiga rawatan (Kawalan, DCR tidak dirawat, dan DCR dirawat) dimodelkan menggunakan lapan algoritma serta model permukaan sambutan kuadratik sebagai asas perbandingan. Model dinilai melalui ramalan terkumpul luar-lipatan di bawah pengesahan K-lipatan rawak, tinggal-satu-campuran-keluar dan tinggal-satu-aras-bitumen-keluar. Bagi campuran AC14, nilai OBC ialah 5.30 % (Kawalan), 4.95 % (tidak dirawat) dan 5.10 % (dirawat). Modulus kenyal, kekuatan tegangan tak langsung (ITS), nisbah kekuatan tegangan (TSR) dan rayapan dinamik diukur dengan setiap campuran yang disediakan pada OBC tersendiri. R^2 terkumpul luar-lipatan mencapai 0.89 bagi lompang terisi bitumen, 0.88 bagi lompang udara, 0.83 bagi ketumpatan pukal, 0.81 bagi lompang dalam agregat mineral, 0.53 bagi aliran dan 0.49 bagi kestabilan. Model permukaan sambutan kuadratik menyamai atau mengatasi model pembelajaran mesin bagi empat daripada enam tindak balas. Di bawah pengesahan tinggal-satu-campuran-keluar, R^2 menjadi negatif bagi kebanyakan tindak balas, manakala pengesahan tinggal-satu-aras-bitumen-keluar mengekalkan R^2 0.47–0.91. Justeru model ini merupakan alat interpolasi dalam ruang reka bentuk yang diuji dan bukan peramal umum. Campuran tidak dirawat memerlukan kandungan pengikat terendah, manakala campuran dirawat mencatat ITS kering tertinggi (1,148.7 kPa) dan TSR tertinggi (50.3 %), walaupun semua campuran berada di bawah had penerimaan TSR lazim.

KEYWORDS: *Asphalt mixture; Marshall mix design; Machine learning; Response surface; Desiccated coconut residue; Indirect tensile strength; Cross-validation*

1. INTRODUCTION

Flexible pavements carry most of the world's paved road traffic, and their service life depends on the mechanical performance of the asphalt concrete (AC) wearing course [1, 2]. Three response variables are commonly used to characterize that performance: the resilient modulus (RM), which reflects the stiffness available to distribute traffic stresses; the indirect tensile strength (ITS), which indicates tensile capacity and moisture-damage susceptibility [5, 6]; and the resistance to permanent deformation under repeated loading, usually evaluated through dynamic creep testing [3, 4]. Each test is reliable but slow, and the Marshall mix design that precedes them adds further effort through its sweep of bitumen contents, replicate specimens, and volumetric calculations [9].

Agricultural and biomass residues have been examined as sustainable bitumen modifiers in Malaysia and elsewhere [33]. Coconut-derived materials are of particular interest because of their local availability; coconut shell and husk powder have been reported to increase binder stiffness and rutting resistance [31, 32]. Desiccated Coconut Residue (DCR), a flaky by-product of commercial coconut-milk production, has received less attention, and its effect on Marshall design properties and on the mechanical performance of the resulting mixtures has not been systematically reported.

Data-driven regression offers a complementary route to reducing laboratory effort. Asi et al. [10] compiled 721 hot-mix asphalt observations and reported R^2 of 0.835 and 0.845 for Marshall stability and flow using CatBoost, with Shapley values identifying aggregate proportion and asphalt content as the principal predictors. Awan et al. [11] applied Multi-

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Expression Programming to 253 base-course and 343 wearing-course specimens and derived explicit equations for stability and flow with training R^2 above 0.90. Kumar et al. [8] compared conventional and hybrid pipelines for plastic-modified asphalt, where neural networks and bagged support-vector variants exceeded correlation coefficients of 0.95 on 195 records. Al-Ammari et al. [12] evaluated several algorithms on a 60-record Marshall dataset and found the neural-network model strongest overall.

The same approach has been extended to fiber- and waste-modified mixtures. Upadhya et al. [24] trained five algorithms on Marshall stability data for glass- and carbon-fiber hybrid asphalt, with Gaussian process regression performing best and fiber content and bitumen percentage jointly governing stability. Jamil et al. [14] applied Random Forest, Gradient Boosting, XGBoost, and a Bagging Regressor to plastic-modified asphalt, obtaining R of 0.95 for training and 0.84 for testing, with SHAP analysis identifying plastic size and bitumen content as dominant. Two findings recur across this literature: bitumen content is the most influential continuous predictor, and non-linear methods outperform linear baselines on volumetric and strength responses.

For the mechanical properties, the resilient modulus measured under repeated indirect tensile loading is a temperature-sensitive stiffness parameter used in mechanistic-empirical design [25]. Shafabakhsh and Tanakizadeh [26] reported marked reductions in resilient modulus between 25 °C and 40 °C, with reduction ratios depending on binder grade and gradation. Indirect tensile strength under the Lottman protocol is the standard moisture-damage screening test, and the wet-to-dry ITS ratio quantifies susceptibility [27, 28]; ratios below roughly 70–80% are conventionally treated as moisture-sensitive [5, 6]. Uniaxial dynamic creep provides cumulative permanent strain and creep stiffness modulus, both of which correlate with wheel-tracking rutting performance [4, 7]. Hussan et al. [3] showed that neural networks reach R^2 up to 0.99 on uniaxial creep data, outperforming non-linear regression on the same records. Reviews of polymer-modified binders report higher resilient modulus at high service temperatures and slower strain accumulation, though the magnitude depends strongly on dosage and base-binder grade [7, 29].

Validation protocol matters more than algorithm choice when the dataset is small [15, 22]. Single train/test splits, still common in pavement machine-learning studies, are sensitive to which records fall in the test partition and yield optimistic estimates that often fail to replicate. Repeated K-fold cross-validation gives a more honest distribution of performance [23], and hyperparameter search must be conducted inside the cross-validation loop to avoid selecting on the test data [15]. Interpretability is commonly addressed through permutation feature importance, which measures the drop in predictive score when a feature is shuffled [19, 22]; its interpretation is affected by correlated or structurally dependent predictors [23], and SHAP values [30] require larger samples than are available here.

Two gaps motivate the present work. First, the published machine-learning literature on asphalt mixtures is dominated by datasets of hundreds to thousands of records, whereas a typical laboratory program produces an order of magnitude fewer observations, and methodological guidance for that regime is sparse. Comparative rankings are also rarely accompanied by a simple physically motivated baseline, so it is seldom clear whether the additional model complexity is justified. Second, mechanical-performance results obtained at the optimum bitumen content are rarely reported alongside the mix-design dataset from which that operating point was derived, even though both inform pavement design [1].

This paper addresses both gaps for DCR-modified asphalt concrete. We model six Marshall responses as functions of bitumen content, treatment condition, and gradation using eight regression algorithms and a quadratic response-surface baseline. Performance is reported as pooled out-of-fold prediction under three validation designs: random K-fold, leave-one-mixture-combination-out, and leave-one-bitumen-level-out. The optimum bitumen content is determined separately for each AC14 mixture, and the resilient modulus, indirect tensile strength, tensile strength ratio, and dynamic-creep response are measured for each mixture at its optimum, so model behavior and laboratory evidence appear in one document. The objective is to establish what such models can and cannot support for practical mix-design decisions.

2. Materials and Experimental Program

2.1. Materials

The additive examined is Desiccated Coconut Residue (DCR), a flaky by-product of commercial coconut-milk production, obtained from Fizah Enterprise, Rawang, Selangor, Malaysia. Two forms were prepared. The untreated form (UT) was oven-dried at 60 °C for 24 hours. The treated form (TR) was oven-dried under the same conditions and then ground for one minute in a high-speed grinder operating at 25,000 rev/min, so that the treated material differs from the untreated material only by the additional grinding step. Particle-size distribution, moisture content, and chemical composition of the DCR were not determined in this program; the study characterizes mixture-level performance rather than additive microstructure, and this restricts mechanistic interpretation of the observed differences.

The base binder was a PEN 60/70 penetration-grade bitumen supplied by K2 Bitumen Sdn. Bhd., selected for the Malaysian climatic range. Measured properties were a penetration of 62.4 dmm at 25 °C (ASTM D5/D5M [34], within the 60–70 dmm range), a softening point of 49 °C (ASTM D36 [35], within the 49–56 °C requirement) and a rotational viscosity of 0.44 Pa·s at 135 °C (ASTM D4402/D4402M [36], below the 3 Pa·s limit). DCR was added at 5 % by mass of the binder for both the UT and TR mixtures, in addition to the binder rather than as a replacement for part of it; the Control mixture used the same binder with no DCR. The 5% dosage was adopted from the preceding phase of the laboratory program, where it produced a workable, homogeneous blend without visible phase separation; the dosage was not varied in the present study. Modified binders were produced by heating 800 g of base binder to 130 °C until pourable, adding the DCR, and mixing for one hour at 160 °C and 1,500 rpm, following a procedure adapted from the biomass-modifier protocol of Mior Sani et al. [33].

Aggregates were supplied by Kajang Rock Quarry, Kajang, Selangor. Coarse fractions of 20, 14, 10, and 5 mm nominal size were blended with fine aggregate to satisfy the JKR gradation envelopes for AC14 (14 mm nominal maximum aggregate size) and AC20 (20 mm) [2]. Hydrated lime was used as the mineral filler throughout, in accordance with JKR requirements, because it improves binder–aggregate adhesion and reduces stripping potential [5, 6]. Aggregate characterization comprised sieve analysis (ASTM C136, AASHTO T27), specific gravity and water absorption (ASTM C127), aggregate crushing value (BS EN 1097-2), Los Angeles abrasion (ASTM C131-81), flakiness index (BS 812; MS 30) and elongation index (ASTM D4791-10), all conducted per the JKR Standard Specification for Road Works [2].

Three treatments were studied for each gradation: a Control mixture without additive, an untreated DCR mixture (UT), and a treated DCR mixture (TR). The full factorial of six gradation-by-treatment mixtures was prepared at five bitumen contents (4, 4.5, 5, 5.5, and 6% by mass of the mixture), with three Marshall replicates per bitumen content, yielding 90 individual specimens and 30 averaged records for volumetric and strength analysis. The optimum bitumen content was determined separately for each AC14 mixture by the Asphalt

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Institute MS-2 averaging procedure, in which the bitumen contents satisfying the individual design criteria (peak density, peak stability, target air voids, target VFB, and flow) are averaged. Table 1 presents the resulting values. Each mixture was then prepared at its own optimum for the mechanical-performance tests. The untreated mixture required the lowest binder content of the three, which is of practical interest because binder is the most costly component of the mixture; a full cost assessment would also need to account for DCR processing and the additional mixing energy, which were not quantified here.

Table 1. Optimum bitumen content determined separately for each AC14 mixture by the Asphalt Institute MS-2 averaging procedure. Mechanical-performance tests were conducted with each mixture prepared at its own optimum.

AC14 mixture	OBC (% by mass of mixture)
Control	5.30
Untreated DCR (UT)	4.95
Treated DCR (TR)	5.10

Mechanical performance testing was confined to the AC14 gradation. The AC20 mixtures were included in the Marshall program, and their mix-design records are therefore retained in the modeling dataset, but resilient-modulus, indirect-tensile, and creep testing of AC20 specimens was not undertaken within the scope and resources of this phase of the laboratory program. AC20 mechanical characterization is planned as a follow-up study. Reporting AC20 mechanical results here would have required a separate optimum-bitumen-content determination that was not performed, and the mechanical comparison is therefore restricted to AC14 so that every mixture compared was tested at its own design point.

2.2. Test methods

Marshall mix-design tests followed the Asphalt Institute MS-2 procedure [9]. For each specimen, 1,200 g of proportioned aggregate was heated to 110–130 °C, mixed with the heated binder until uniformly coated, placed in a preheated mould, and compacted with 75 blows per face. After cooling and extrusion, specimens were conditioned in a water bath at 60 °C for 30 minutes before stability and flow measurement. Air voids and VMA were computed from the maximum theoretical specific gravity and the bulk density obtained from saturated surface-dry weighings.

Resilient modulus was measured on a universal testing machine per ASTM D7369-20 [25], using an indirect tensile loading fixture and linear variable differential transformers for horizontal deformation. Repeated haversine pulses were applied along the diametral axis with the load level set to keep the response within the recoverable strain range. One specimen per treatment was tested, and that specimen was measured first at 25 °C and then at 40 °C; the two temperature results are therefore repeated measurements on the same specimen rather than independent replicates. The resilient modulus was taken as the ratio of applied stress to recoverable strain averaged over stable cycles.

Indirect tensile strength followed ASTM D6931 [38] with moisture conditioning per AASHTO T283 [27]. Specimens were compacted to a target air-void level of 7 ± 1 %. The conditioned subset was vacuum saturated to 70–80 % degree of saturation, held in a water bath at 60 °C for 24 hours, and then brought to 25 °C for one hour before testing; no freeze–thaw cycle was applied. Dry and conditioned specimens were loaded diametrically at 50 mm/min to

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failure, and the tensile strength ratio was computed as the ratio of the mean conditioned to the mean dry strength. Two replicates were tested in each condition.

Dynamic creep was performed as a uniaxial repeated-load cyclic compression test per EN 12697-25 [37] on cylindrical specimens of nominal length 70 mm and diameter 100 mm, with 3,600 haversine cycles at 40 °C, the temperature at which rutting is most critical [3, 4]. Two specimens per treatment were tested.

Table 2. Variables used in the study and their role in the modeling and experimental analyses.

Variable	Symbol	Unit	Role	Notes
Bitumen content	BC	% by mass of mix	Model input	5 levels: 4.0–6.0 %
Treatment	—	categorical	Model input	Control (reference)
Gradation	—	categorical	Model input	AC14 (reference) /
Bulk density	ρ	g/cm³	Target	Marshall response
Marshall stability	S	kN	Target	Marshall response
Marshall flow	F	mm	Target	Marshall response
Air voids	Va	%	Target	Marshall response
Voids in mineral	VMA	%	Target	Marshall response
Voids filled with	VFB	%	Target	Marshall response
Resilient modulus	MR	MPa	Reported only	AC14, 3 specimens,
Indirect tensile	ITS	kPa	Reported only	AC14, 12
Tensile strength	TSR	%	Reported only	AC14, derived per
Permanent strain @	ε(3600)	%	Reported only	AC14, 4 specimens

Table 3. Composition of the experimental datasets and their role in the analysis. The mechanical datasets are reported descriptively; their sample sizes do not support cross-validated regression.

Dataset	Records	Inputs	Targets	Use
Marshall (bitumen	30 averaged (from	bitumen content,	6 Marshall	Regression
Resilient modulus	3 specimens × 2	treatment,	MR	Reported
Indirect tensile	12 (3 mixtures × 2	treatment, condition	ITS, TSR	Reported
Dynamic creep	4 accepted	treatment	ε(1200), ε(3600),	Reported

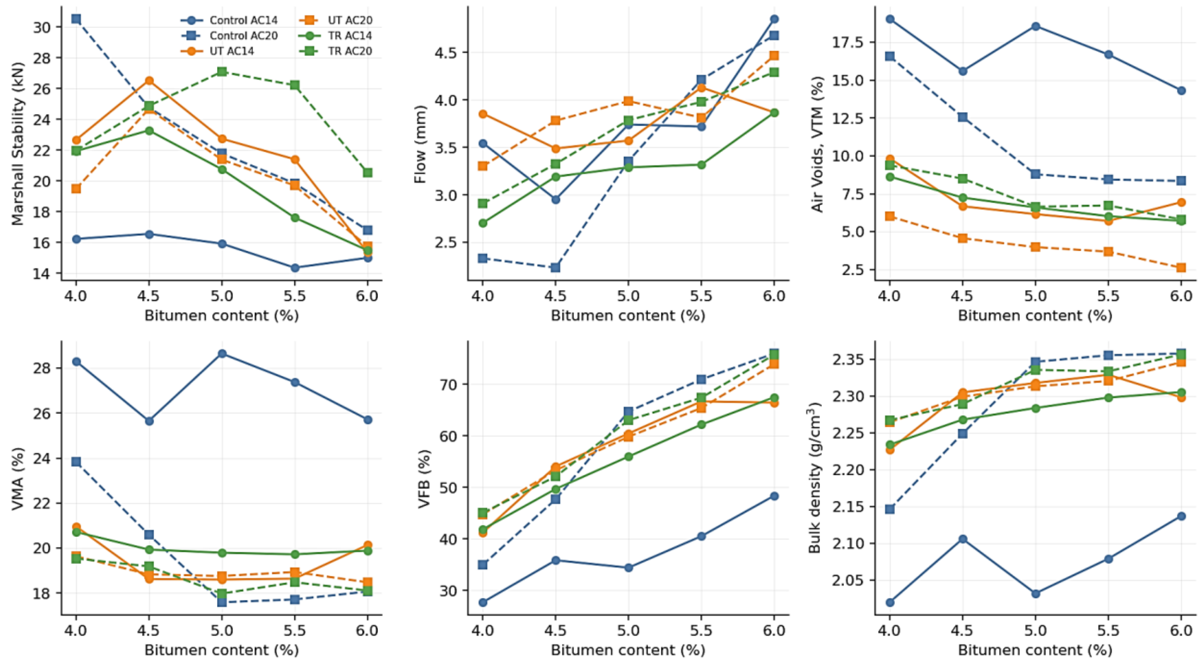

Figure 1. Marshall mix-design responses against bitumen content for the six mixtures (Control, untreated DCR, treated DCR; gradations AC14 and AC20). Each curve traces five bitumen-content levels at the averaged-replicate level. The Control AC14 mixture shows the highest VMA and the lowest density across the bitumen range; both DCR mixtures shift the density curve upwards and the air-voids curve downwards.

3. Modeling Methodology

The modeling dataset comprises the 30 averaged Marshall records: six mixture combinations (two gradations × three treatments) at five bitumen contents. Each record is the mean of three replicate specimens, which is the level at which Marshall design curves are conventionally reported. Averaging reduces within-condition experimental scatter, so the models predict mean mixture-condition responses rather than specimen-level variability, and the reported accuracies are correspondingly more favorable than specimen-level modeling would give. The three inputs are bitumen content (continuous), treatment, and gradation. Both categorical inputs are encoded with a reference category dropped: Control for treatment and AC14 for gradation, which avoids exact collinearity with the fitted intercept. Each of the six responses is modeled as a separate regression problem.

Nine models were compared: ordinary least squares, which is unregularized; three regularized linear models, namely Ridge, Lasso, and Elastic Net [16, 17]; support vector regression with a radial basis kernel [18, 39]; three tree ensembles, namely Random Forest, Extra Trees and Gradient Boosting [19, 20, 21]; and a quadratic response-surface model consisting of second-degree polynomial features with ridge regularization. The response surface is included as a physically motivated baseline, because Marshall responses are expected to vary non-linearly with bitumen content, and it provides a reference against which the value of the machine-learning models can be judged. We encapsulate preprocessing that depends on the data distribution in a pipeline so fitting occurs only within training folds [23]. Hyperparameter grids and the selected values are given in the Appendix.

We used three validation designs and compute all metrics from pooled out-of-fold predictions rather than averaging fold-level scores. With only six records in a test fold, fold-level R^2 is unstable because it depends on the target variance that happens to fall in that fold; pooling the out-of-fold predictions before computing the metric avoids this artifact and is more interpretable. The first design is repeated random 5-fold cross-validation, with five repeats using different random seeds. The second is leave-one-mixture-combination-out validation, in which all five records of one gradation–treatment combination are held out together, so the model must predict a mixture it has never seen. The third is leave-one-bitumen-level-out validation, in which all six records at one bitumen content are held out together, so the model must predict an unobserved binder level. Hyperparameter search is repeated inside the training partition of every outer fold in all three designs. The coefficient of determination, root-mean-square error, and mean absolute error are reported for each.

Random K-fold splitting assigns records from the same mixture curve to both the training and test partitions, so it measures interpolation within the observed factorial rather than generalization to new mixtures. The two grouped designs were added specifically to separate these two questions, and the contrast between them is central to the interpretation offered in Section 4.

4. Results and Discussion

4.1. Dataset Characteristics

Descriptive statistics for the six responses across the 30 averaged records are given in Table 4. Bulk density ranges from 2.02 g/cm³ for the Control AC14 mixture at 4 % bitumen to 2.358 g/cm³ for the AC20 TR mixture at 6 %. Marshall stability spans 14.4–30.5 kN, and flow spans 2.23–4.85 mm. Air voids vary widely, from 2.62% to 19.03%, and this spread reflects both bitumen-content and treatment effects. VMA spans 17.6–28.6 % and VFB 27.7–76.0 %. The correlation structure in Figure 2 shows near-perfect negative correlations between density and VMA and between density and air voids, which follow from the volumetric definitions rather than from independent observation. Bitumen content correlates positively with flow (+0.74) and VFB (+0.76) and negatively with stability (−0.51), consistent with the expected unimodal stability curve [9].

Table 4. Descriptive statistics for the input variable and the six target responses across the 30 averaged Marshall records.

Variable	n	Mean	SD	Min	Median	Max
Bitumen	30	5.00	0.72	4.00	5.00	6.00
Bulk density	30	2.261	0.097	2.020	2.298	2.358
Stability (kN)	30	20.71	4.20	14.36	21.07	30.52
Flow (mm)	30	3.62	0.62	2.23	3.73	4.85
Air voids (%)	30	8.88	4.53	2.62	7.10	19.03
VMA (%)	30	20.62	3.25	17.60	19.59	28.65
VFB (%)	30	54.94	13.50	27.71	55.03	76.00

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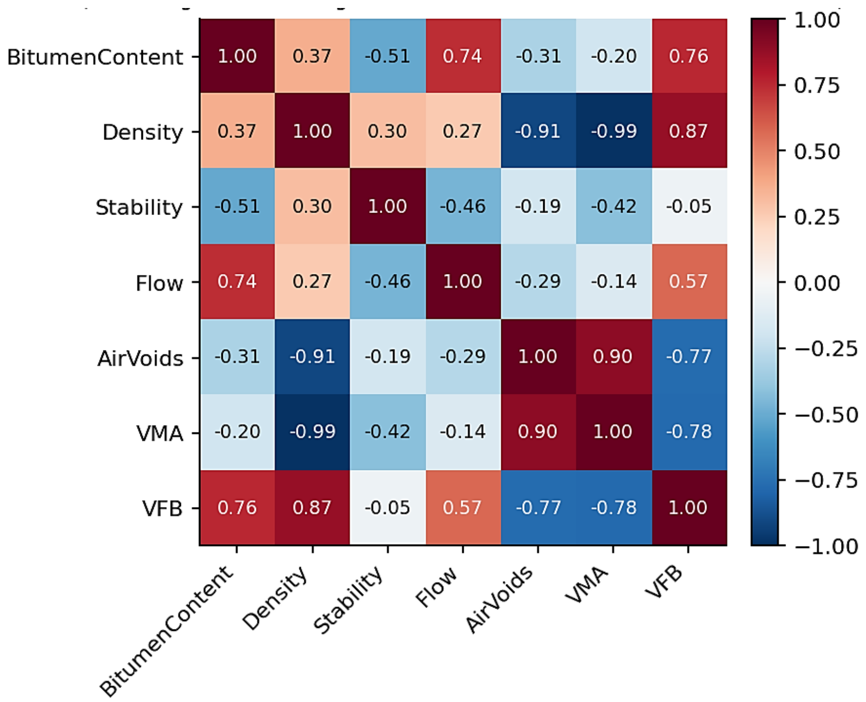

Figure 2. Pearson correlation matrix of the six Marshall design variables and bitumen content. The strong negative correlations between density and air voids and between density and VMA follow from the volumetric definitions rather than from independent measurement.

4.2. Predictive Performance and What It Supports

Table 5 reports pooled out-of-fold performance for the best model of each response under all three validation designs. Under random K-fold validation, the volumetric responses are predicted well: R^2 of 0.89 for VFB, 0.88 for air voids, 0.83 for density, and 0.81 for VMA. Flow reaches 0.53 and stability 0.49. These values are markedly higher than would be obtained by averaging fold-level R^2, which, for the flow response, yields a near-zero value purely because individual six-record folds contain little flow variance. The pooled estimates are defensible, and the difference illustrates why the choice of metric matters at this sample size.

Table 5. Pooled out-of-fold performance of the best model for each Marshall response under three validation designs. RMSE and MAE correspond to the random K-fold design and are expressed in the units of each response. Results for all nine models are given in the Appendix.

Response	Best model	Random K-	RMSE	MAE	Leave-one-	Leave-one-
Bulk density (g/cm^3)	Response surface	0.826	0.039	0.029	−4.43	0.838
Stability (kN)	SVR (RBF)	0.487	2.896	2.227	−0.15	0.610
Flow (mm)	Response surface	0.528	0.415	0.326	0.00	0.467
Air voids (%)	Response surface	0.879	1.535	1.151	−1.23	0.882
VMA (%)	Response surface	0.812	1.359	1.026	−4.00	0.822
VFB (%)	SVR (RBF)	0.895	4.261	3.572	0.23	0.881

The most consequential result in Table 5 is the contrast between the two grouped designs. Under leave-one-bitumen-level-out validation, where the model must predict an unobserved binder content for mixtures it has otherwise seen, performance is retained across all six responses (R^2 of 0.47–0.88). Under leave-one-mixture-combination-out validation, where an entire gradation–treatment combination is withheld, R^2 becomes negative for four of the six responses, meaning the models perform worse than predicting the training mean. The models interpolate competently along the bitumen-content axis but carry essentially no ability to predict a mixture family they have not encountered. This is a direct consequence of the design: with three treatments and two gradations, withholding one combination removes the only evidence the model has about that category. The practical implication is specific. These models can reduce laboratory effort by predicting intermediate binder contents for a mixture whose Marshall behavior has been partially characterized, as in optimum-bitumen-content determination, but they cannot be used to screen a new additive or gradation without fresh testing.

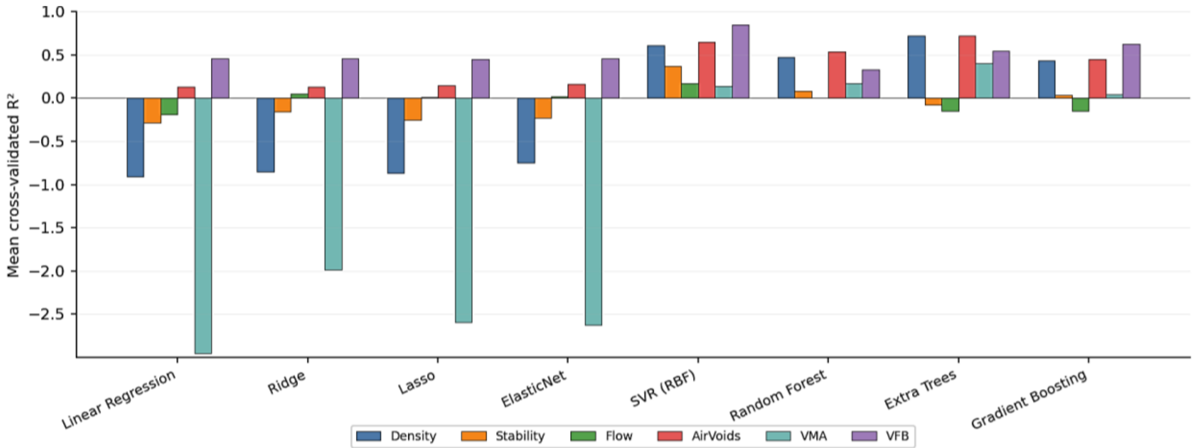

Figure 3. Cross-validated R^2 across the candidate algorithms for each Marshall response under random K-fold validation. Linear baselines trail the kernel, ensemble, and response-surface methods on all six responses.

The quadratic response surface is the best-performing model for density, flow, air voids, and VMA, and it is within 0.01 R^2 of the best model for VFB. Support vector regression retains an advantage only for stability and VFB. This is a useful negative result. The machine-learning algorithms do not deliver a material improvement over a second-degree polynomial in bitumen content combined with treatment and gradation indicators, and for a design space of this size the response surface is preferable for transparency, since its coefficients can be inspected and reported directly. Ordinary least squares, which lacks polynomial terms, performs substantially worse (R^2 of 0.18–0.77), confirming that the curvature rather than the algorithm family is what matters. The classical Marshall stability response peaks near the optimum and declines on either side [9], and any model without curvature in the bitumen content cannot reproduce that shape.

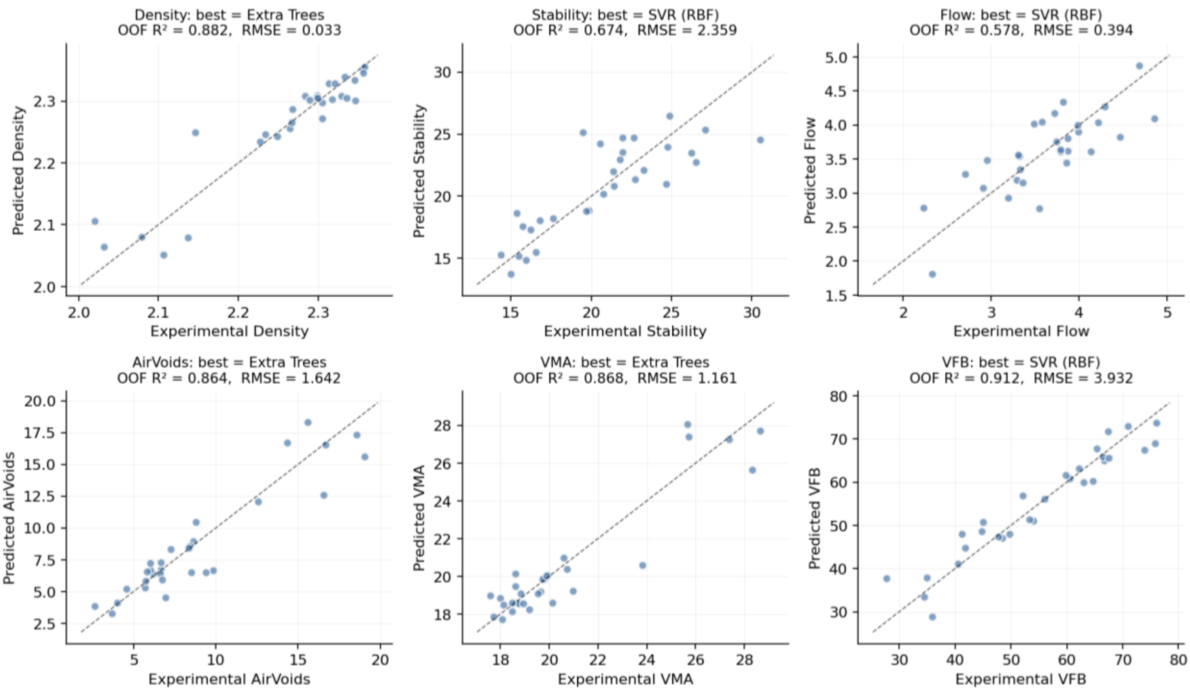

Figure 4. Out-of-fold predictions against experimental values for each Marshall response using the best model per response. Predictions are pooled across one 5-fold partition, giving one point per record.

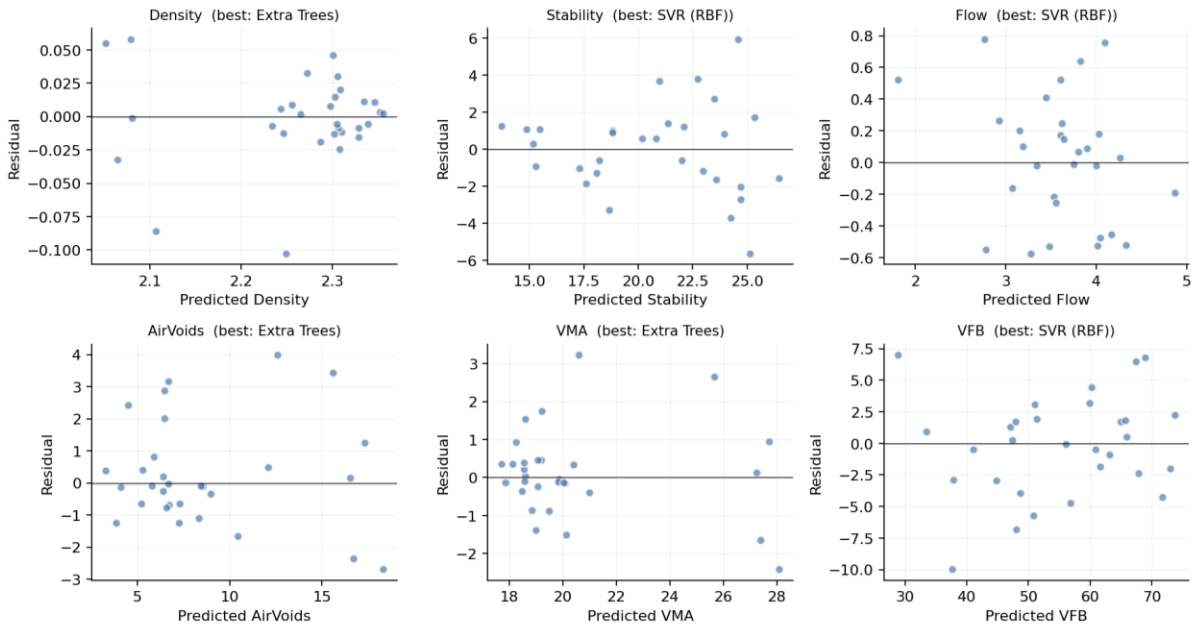

Figure 5. Residuals against predicted values for the best model of each response. Residuals center near zero for all responses; the wider scatter for stability and VFB at the extremes of their ranges reflects the greater experimental variability at the low-bitumen end of the design.

4.3. Feature Importance

Figure 6 shows permutation importance computed on the fitted models. Bitumen content dominates for stability and VFB, consistent with its established mechanistic role [10, 11]. For density, air voids, and VMA, the treatment indicator separating the Control mixture from the two DCR mixtures dominates. This reflects a categorical separation in the experimental design rather than a dose-response effect: DCR was applied at a single dosage, so the model can only distinguish presence from absence, and the Control mixture is volumetrically distinct from the two DCR mixtures, which cluster together. Because treatment was encoded categorically and dosage did not vary, these results identify predictive separations within the studied design and cannot be read as evidence of a physical mechanism by which DCR alters density. Establishing a dose-response relationship would require multiple DCR dosages [8, 14]. The importance values are also computed from models fitted on the full dataset, which makes them descriptive rather than an unbiased estimate of predictive contribution.

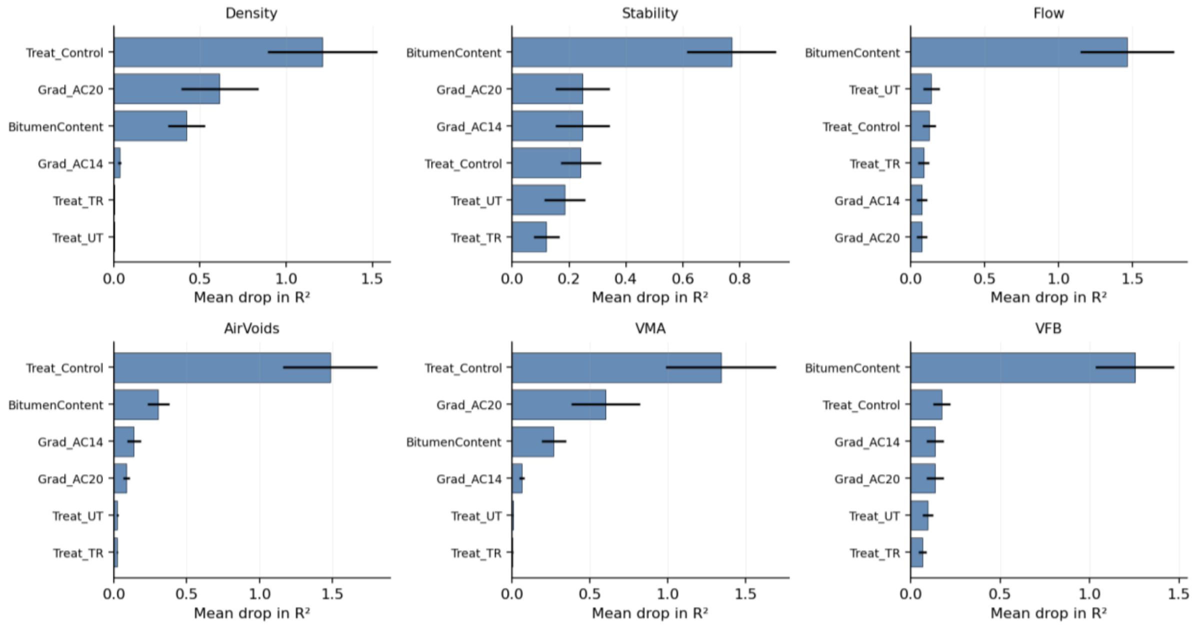

Figure 6. Permutation feature importance for each Marshall response. Bars give the mean reduction in R^2 when a feature is shuffled; error bars are the standard deviation across 50 repeats. Values are descriptive and should not be interpreted as evidence of a physical DCR mechanism.

4.4. Mechanical Performance at the Optimum Bitumen Content

The resilient modulus, indirect tensile strength, and creep results are reported as direct measurements without regression modeling or an associated R^2. This is deliberate. Each property was measured only at the optimum bitumen content of each mixture, giving three resilient-modulus specimens, twelve indirect-tensile measurements, and four accepted creep specimens. Cross-validated R^2 estimated from samples of this size would be dominated by the chosen partition rather than any underlying response surface, and reporting such values would misrepresent the strength of the evidence. Because only two replicates are available per condition, the comparisons below are descriptive, and the differences reported are not supported by statistical tests.

Table 6 gives the resilient modulus at 25 °C and 40 °C. At 25 °C, the three mixtures fall within a narrow band of 11,815–12,646 MPa, with the untreated mixture highest and the Control 6.6 % below it. At 40 °C, the modulus falls by 62–74 %, which is consistent with the temperature sensitivity of the binder reported in the literature [26, 29], and the Control mixture retains the highest value. The treated mixture shows the largest proportional reduction. With one specimen per treatment and the two temperatures measured on that same specimen, these values are point measurements, and the ordering between mixtures should not be regarded as established.

Table 6. Resilient modulus of the AC14 mixtures, each tested at its own optimum bitumen content. One specimen per treatment was measured at both temperatures, so the two columns are repeated measurements on the same specimen.

Treatment	MR at 25 °C (MPa)	MR at 40 °C (MPa)	Reduction (%)
Control	11,815	4,488	62.0
Untreated DCR (UT)	12,646	3,878	69.3
Treated DCR (TR)	12,039	3,147	73.9

Indirect tensile strength results are given in Table 7. The treated mixture recorded the highest dry strength (1,148.7 kPa) and the highest conditioned strength (577.4 kPa), both above the corresponding Control values (945.9 and 455.6 kPa). The Control and untreated mixtures recorded closely similar strengths in both conditions, which suggests that grinding rather than the presence of DCR is associated with the strength difference, although with two replicates per condition this observation is descriptive. Tensile strength ratios were 48.2% for the Control, 47.6% for the untreated mixture, and 50.3% for the treated mixture, all well below the 70–80% range commonly adopted as an acceptance criterion [5, 6, 27].

Table 7. Indirect tensile strength of the AC14 mixtures, each tested at its own optimum bitumen content. Means and standard deviations are computed across two replicate specimens per condition.

Treatment	ITS dry (kPa, mean ± SD)	ITS conditioned (kPa, mean ± SD)	TSR (%)
Control	945.85 ± 5.45	455.64 ± 44.72	48.2
Untreated DCR (UT)	955.54 ± 82.01	454.87 ± 34.87	47.6
Treated DCR (TR)	1,148.72 ± 29.66	577.38 ± 14.74	50.3

That all three mixtures fell below common acceptance limits despite the use of hydrated lime as filler is the most practically significant result of the experimental program, and it warrants comment. Hydrated lime is specified precisely because it promotes binder–aggregate adhesion and reduces stripping [5, 6], so its presence would ordinarily be expected to lift the tensile strength ratio. Three explanations fit the data. First, the conditioned specimens lost roughly half their dry strength, a reduction characteristic of adhesive failure at the binder–aggregate interface rather than cohesive failure within the binder, pointing to the interface as the controlling weakness. Second, the granite-derived aggregate used here is siliceous and therefore intrinsically hydrophilic, and lime alone may be insufficient to compensate for that in a wearing course subjected to a full 24-hour saturated conditioning cycle. Third, DCR is an organic residue with residual moisture affinity, and its presence at the interface may itself provide pathways for water ingress; the treated form, which was ground more finely, gave the highest ratio of the three, which is at least consistent with better dispersion reducing such pathways. Distinguishing these mechanisms would require interface-level characterization that was not part of this program. For practical purposes, the implication is that DCR-modified mixtures of this type should not be specified for moisture-exposed applications on the basis of lime filler alone; a liquid anti-stripping agent, a higher lime dosage, or a less hydrophilic aggregate source would need to be evaluated, and drying the DCR to a lower residual moisture content before blending may also be worth testing.

Table 8 presents the dynamic-creep results for the four accepted AC14 specimens. The Control specimens accumulated a mean permanent strain of 2.57 % at 3,600 cycles against 2.15 % for the treated specimens, and the mean creep stiffness modulus was 79.4 MPa for the Control and 60.9 MPa for the treated mixture. The two indicators therefore do not order the mixtures consistently, and with two specimens per treatment, no conclusion about relative rutting resistance is supported. The individual strain histories in Figure 8 show the divergence directly: specimen TR14-S1 accumulated approximately 25,000 με by cycle 3,600 while TR14-S2 reached roughly 14,000 με, a spread wider than the difference between the treatment means.

Table 8. Dynamic Creep Results and Untreated Specimen Exclusion

Specimen	Treatment	ε(1200) %	ε(3600) %	CSM (MPa)
C14-S1	Control	2.174	2.467	102.4
C14-S2	Control	2.131	2.663	56.4
TR14-S1	Treated DCR	2.303	2.969	45.0
TR14-S2	Treated DCR	0.930	1.321	76.7

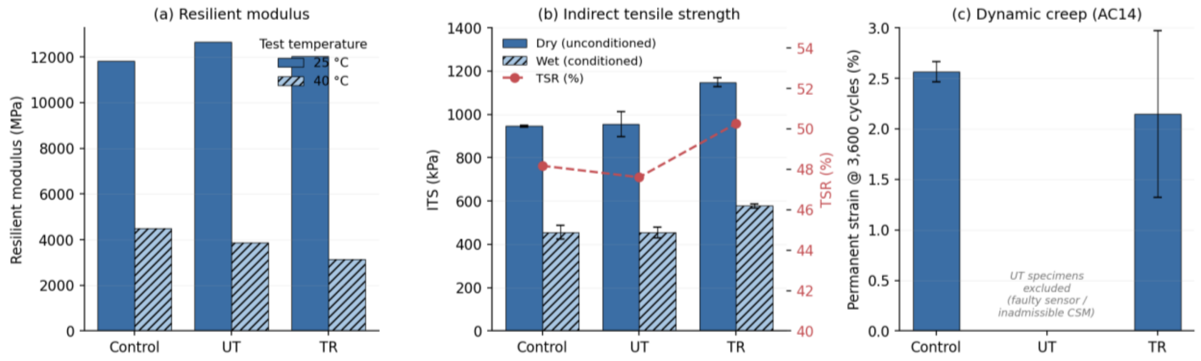

Figure 7. Mechanical performance of AC14 mixtures at optimum bitumen content: (a) resilient modulus at 25 °C and 40 °C; (b) dry and conditioned indirect tensile strength with tensile strength ratio; and (c) permanent strain at 3,600 cycles. Untreated specimens were excluded during data-quality screening (Table 8).

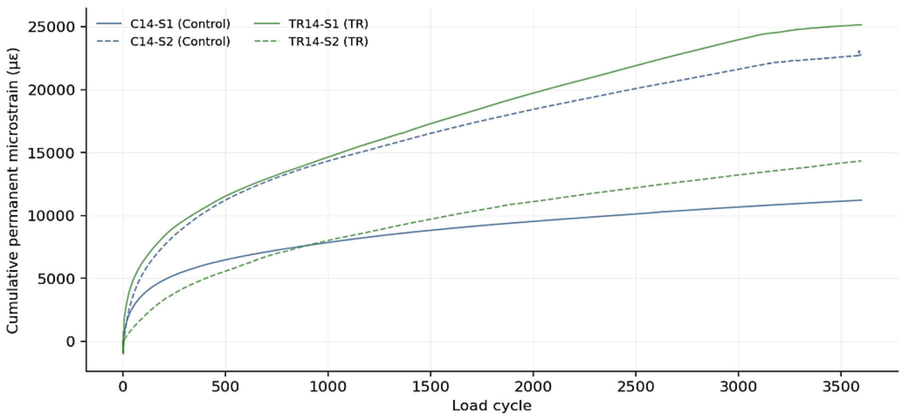

Figure 8. Cumulative permanent microstrain versus load cycles for accepted AC14 creep specimens. Control specimens showed typical primary–secondary creep, while treated specimens diverged, reaching approximately 25,000 and 14,000 με at 3,600 cycles.

4.5. Synthesis and Scope of the Findings

Taken together, the modeling and experimental results point in the same direction. The regression models reproduce the volumetric responses well because those responses vary smoothly and largely deterministically with binder content within a given mixture; the same smoothness is visible in the Marshall curves of Figure 1. Stability and flow are predicted less well because they depend on mechanical behavior that the three available inputs do not capture, and the mechanical tests show why: at a fixed binder content, the three mixtures differ in tensile strength and creep response in ways that bitumen content, treatment category, and gradation cannot express. The information needed to predict mechanical response is not present in mix-design variables alone.

The scope of what these models support is correspondingly narrow. They are interpolation tools for the tested design space. Within that space, they can reduce the number of trial bitumen contents required during optimum-content determination, which is a real, if modest, saving of laboratory effort. They cannot predict performance for an untested additive, dosage, or gradation, as the leave-one-mixture-out results show plainly. They also cannot substitute for the mechanical tests: no relationship established here would have predicted that all three mixtures fail the tensile strength ratio criterion, which is the finding with the clearest bearing on whether these mixtures could be used in practice. Extending the models beyond interpolation would require a dataset spanning several DCR dosages, multiple aggregate sources, and specimen-level rather than averaged records, together with mechanical testing at more than one binder content so that the mechanical responses themselves become modellable.

5. CONCLUSIONS

This study evaluated regression models for six Marshall mix-design responses of DCR-modified asphalt concrete and characterized the mechanical performance of the modified AC14 mixtures at their respective optimum bitumen contents. The following conclusions are drawn.

The optimum bitumen content differed between mixtures: 5.30% for the Control, 4.95% for the untreated DCR mixture, and 5.10% for the treated DCR mixture. The untreated mixture therefore required the least binder, which is relevant to mixture cost, although a complete assessment would need to include the cost of processing the additive.

Pooled out-of-fold coefficients of determination under random K-fold validation were 0.89 for voids filled with bitumen, 0.88 for air voids, 0.83 for bulk density, 0.81 for voids in mineral aggregate, 0.53 for flow, and 0.49 for stability. Volumetric responses are therefore predictable from bitumen content, treatment, and gradation, whereas the mechanically governed responses are only partially so.

A quadratic response surface matched or exceeded the machine-learning algorithms on four of the six responses. For a design space of this size, the additional complexity of the machine-learning models is not warranted, and the response surface is preferable because its coefficients can be inspected directly.

Validation design determines what the reported accuracy means. When an entire mixture combination was withheld, the coefficient of determination became negative for four of six responses, whereas withholding a bitumen level retained values of 0.47 to 0.88. The models are interpolation tools within the tested design space and cannot predict the behavior of an untested mixture family.

Among the mechanical properties, the treated DCR mixture recorded the highest dry and conditioned indirect tensile strength. All three mixtures returned tensile strength ratios between

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47.6% and 50.3%, well below common acceptance limits, despite using hydrated lime as a mineral filler. On this evidence, DCR-modified mixtures of the type tested here require additional anti-stripping measures before they could be considered for moisture-exposed applications.

Further work should extend the experimental matrix across several DCR dosages, characterize the additive itself, repeat the untreated-mixture creep tests that were excluded here, increase replication so that differences in mechanical performance can be tested statistically, and conduct the mechanical tests at more than one binder content so that those responses become amenable to modeling in their own right.

DATA AVAILABILITY

The 30-record modeling dataset, the descriptive experimental results reported in Tables 6 to 8, the complete model-comparison results for all nine algorithms and three validation designs, the analysis code including preprocessing pipeline and hyperparameter grids, and the raw traces of the excluded creep specimens are available from the corresponding author on reasonable request. The analysis was performed in Python 3.12 with scikit-learn 1.8, NumPy 2.4, and pandas 3.0. A fixed random seed of 42 was used for all cross-validation partitioning and model fitting, so that reported results are reproducible.

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APPENDIX A. MODEL SPECIFICATIONS AND FULL RESULTS

Hyperparameter grids were searched by exhaustive grid search within the training partition of every outer fold. Ridge regularisation strength was searched over {0.01, 0.1, 1, 10, 100}; Lasso over {0.001, 0.01, 0.1, 1}; Elastic Net over the same alpha values with l1 ratios of {0.2, 0.5, 0.8}. Support vector regression used $C \in \{0.1, 1, 10, 100\}$, $\varepsilon \in \{0.01, 0.1, 0.5\}$ and $\gamma \in$ {scale, 0.1, 1.0}. Random Forest and Extra Trees used 200 estimators with maximum depth $\in$ {none, 4} and minimum samples per leaf $\in \{1, 2\}$. Gradient Boosting used 200 estimators with learning rate $\in \{0.05, 0.1\}$ and maximum depth $\in \{2, 3\}$. The response-surface model used second-degree polynomial features with a ridge penalty searched over {0.001, 0.01, 0.1, 1, 10}.

Table A1. Pooled out-of-fold coefficient of determination for representative models under the three validation designs. Complete results for all nine models, including root-mean-square and mean absolute errors and the hyperparameters selected in each fold, are available from the corresponding author.

Response	Model	Random K-fold R^2	Leave-one-mixture-out R^2	Leave-one-bitumen-level-out R^2
Density	OLS	0.513	−1.11	0.603
Density	SVR (RBF)	0.823	−0.76	0.754
Density	Extra Trees	0.744	−1.60	0.808
Density	Response surface	0.826	−4.43	0.838
Stability	OLS	0.176	−1.09	0.167
Stability	SVR (RBF)	0.487	−0.15	0.610
Stability	Extra Trees	0.153	−0.81	0.336
Stability	Response surface	0.297	−0.83	0.326
Flow	OLS	0.426	−0.04	0.397
Flow	SVR (RBF)	0.467	0.31	0.255
Flow	Extra Trees	0.293	0.17	0.496
Flow	Response surface	0.528	0.00	0.467
Air voids	OLS	0.773	0.13	0.788
Air voids	SVR (RBF)	0.819	0.09	0.739
Air voids	Extra Trees	0.840	−0.74	0.874
Air voids	Response surface	0.879	−1.23	0.882
VMA	OLS	0.460	−1.34	0.558
VMA	SVR (RBF)	0.764	−0.77	0.704
VMA	Extra Trees	0.780	−1.87	0.840
VMA	Response surface	0.812	−4.00	0.822
VFB	OLS	0.738	−0.03	0.791
VFB	SVR (RBF)	0.895	0.23	0.881
VFB	Extra Trees	0.537	−0.08	0.753
VFB	Response surface	0.885	−1.38	0.913

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