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Regression Modeling for the Formulation Optimization of a Stabilizing Additive for Stone Mastic Asphalt

A. A. Afanasenka[1], P. P. Yatsevich[1]

[1]Belarusian National Technical University (Minsk, Republic of Belarus)

Abstract. This study addresses the urgent issue of improving the durability of Stone Mastic Asphalt pavements, where a key technological challenge is binder drainage at high manufacturing temperatures. Existing solutions based on costly imported stabilizing additives create significant economic barriers to their widespread use. The objective of this research was to develop and scientifically validate an optimal formulation for a cost-effective composite stabilizing additive based on locally available raw materials, including cellulose fiber from waste paper and polymer fiber from industrial waste. To solve this multifactorial optimization problem, the method of multiple regression analysis was employed. The experimental basis for the modeling was derived from laboratory tests on 16 additive formulations with varying component proportions. The independent variables (factors) included the percentages of synthetic fiber, cellulose, and a thermal stabilizer, as well as the final dosage of the additive in the asphalt mix. The dependent variables (responses) were key performance indicators such as binder drainage, tensile strength at 0 °C, and compressive strength at 50 °C. As a result of the study, three linear regression models describing the "composition-property" relationships were developed. The high predictive capability of the models was confirmed by statistical metrics; the coefficient of determination R^2 for all equations exceeded 0.90, indicating a high degree of explained variance. Based on these models, an optimization problem with specified criteria and constraints was solved, allowing for the analytical determination of the optimal ranges for component content. Verification of the predictions against strong agreement showed a nearly perfect match between calculated and experimental data. A scientifically validated and patented final additive composition was developed, which ensures compliance with asphalt concrete standards and serves as a competitive alternative to existing analogues.

Keywords: Stone Mastic Asphalt (SMA), stabilizing additive, binder drainage, industrial waste, regression analysis, mathematical modeling, formulation optimization

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Регрессионное моделирование в задаче оптимизации рецептуры стабилизирующей добавки для щебеночно-мастичного асфальтобетона

А. А. Афанасенко[1], П. П. Яцевич[1]

[1]Белорусский национальный технический университет (Минск, Республика Беларусь)

Реферат. Актуальность исследования обусловлена необходимостью повышения долговечности дорожных покрытий из щебеночно-мастичного асфальтобетона, ключевой технологической проблемой при производстве которого является стекание битумного вяжущего при высоких температурах. Существующие решения, основанные на применении дорогостоящих импортных стабилизирующих добавок, создают значительные экономические барьеры для их широкого внедрения. Целью настоящей работы являлись разработка и научное обоснование оптимальной рецептуры экономически эффективной композиционной стабилизирующей добавки на основе доступного местного сырья, включающего целлюлозное волокно из макулатуры и полимерное волокно из промышленных отходов. Для решения поставленной многофакторной оптимизационной задачи был применен метод множественного регрессионного анализа. Экспериментальной базой для моделирования послужили результаты лабораторных испытаний 16 составов

Адрес для переписки
Афанасенко Алексей Александрович
Белорусский национальный технический университет
просп. Независимости, 65,
220013, г. Минск, Республика Беларусь
Тел.: +375 29 338-78-40
CNIIDSGM@bntu.by

Address for correspondence
Afanasenka Aliaksei A.
Belarusian National Technical University
65, Nezavisimosty Ave.,
220013, Minsk, Republic of Belarus
Tel.: +375 29 338-78-40
CNIIDSGM@bntu.by

добавки с варьируемым содержанием компонентов. В качестве независимых переменных (факторов) рассматривались процентные доли синтетического волокна, целлюлозы, термостабилизатора, а также итоговая дозировка добавки в асфальтобетонной смеси. В качестве зависимых переменных (откликов) были выбраны ключевые эксплуатационные показатели, такие как стекание вяжущего, предел прочности при растяжении при 0 °С и предел прочности при сжатии при 50 °С. В результате исследования были построены три линейные регрессионные модели, описывающие зависимости «состав – свойство». Высокая прогностическая способность моделей подтверждена статистическими метриками. Коэффициент детерминации R^2 для всех уравнений превысил 0,90, что свидетельствует о высокой степени объясненной дисперсии. На основе полученных моделей была решена задача оптимизации с заданными критериями и ограничениями, что позволило аналитически определить оптимальные диапазоны содержания компонентов. Верификация прогнозов на контрольных составах показала практически полное совпадение расчетных и экспериментальных данных. Научно обоснован и запатентован итоговый состав добавки, обеспечивающий нормативные показатели асфальтобетона и являющийся конкурентоспособной альтернативой аналогам.

Ключевые слова: щебеночно-мастичный асфальтобетон (ЩМА), стабилизирующая добавка, стекание вяжущего, промышленные отходы, регрессионный анализ, математическое моделирование, оптимизация состава

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Introduction and research objective

One of the key technologies aimed at improving the operational reliability and durability of road pavements is the use of stone mastic asphalt. Its frame structure, formed from high-strength cubical crushed stone, combined with a high content of bituminous binder, provides high resistance to rutting and the effects of climatic factors. However, this advantage is associated with a critical technological limitation, the tendency of the asphalt mixture to segregate and drain the binder at high production and laying temperatures. This phenomenon leads to a violation of the homogeneity of the material structure and, as a consequence, to a decrease in its durability.

The traditional solution to this problem is the introduction of special stabilizing additives, usually of a fibrous nature, into the mixture. Today, the market is dominated by granulated additives based on imported cellulose, the cost of which significantly increases the cost of asphalt concrete. In the context of the need for import substitution and cost optimization in road construction, as well as within the framework of the concept of sustainable development, the scientific task of creating alternative stabilizers is becoming relevant. A promising direction is the development of composite additives based on available local raw materials, including with the involvement of industrial waste in the economic turnover.

The purpose of this study is to develop and scientifically substantiate the optimal formulation of such a multicomponent stabilizing additive. The scientific hypothesis is that the complex relationships between the composition of the additive and the physical and mechanical properties of asphalt concrete can be described with high accuracy by mathematical models. This approach allows moving from the empirical method of component selection to a targeted analytical search for the optimal solution. The method of multiple regression analysis, which has proven its effectiveness in solving similar multifactorial problems in materials science, was chosen as the main tool for testing the hypothesis and achieving the set goal.

Analysis of the current state of the issue

The introduction of fibrous additives is a widely studied and applied in practice method for modifying the properties of asphalt mixtures. An analysis of modern scientific literature shows that fibers in asphalt concrete perform two main, but distinct, roles: stabilization and reinforcement [1, 2, 3]. The first function is to stabilize the asphalt mixture, which is especially critical for compositions with a high binder content, such as stone mastic asphalt. The second function is to reinforce the asphalt concrete matrix in order to improve its mechanical characteristics and increase durability.

To perform the stabilizing function, which consists in preventing the drainage of the binder, natural fibers, primarily cellulose, have found the widest application. Studies also confirm the effectiveness of natural fibers, for example, sisal, coconut, jute, bamboo and others [4–11]. However, the dominant position of cellulose fibers in industrial applications is due to a combination of technological and economic factors. A developed industrial base for the processing of wood and waste paper ensures their mass availability and economic feasibility. An important aspect is also the high degree of product standardization. Industrial methods for producing cellulose make it possible to produce fiber with stable and predictable physical characteristics, such as geometry and purity, which is critically important for ensuring the quality of the asphalt mixture. These factors, in combination with many years of successful application experience, have secured for cellulose the status of a basic and most studied component for solving the stabilization problem [12, 13].

The reinforcing function is aimed at improving the complex of mechanical properties of asphalt concrete, including resistance to fatigue failure, rutting and low-temperature cracking. For this purpose, synthetic polymer fibers, such as polyester, polypropylene or aramid, are mainly used [14–19]. Possessing high tensile strength and modulus of elasticity, they form a spatial reinforcing frame in the volume of asphalt concrete. This three-dimensional network contributes to a more effective redistribution of internal stresses from traffic and temperature effects, slowing down the nucleation and propagation of microcracks.

The analysis shows that for a comprehensive improvement of the properties of asphalt concrete, a scientifically sound approach is the creation of composite additives that combine stabilizing and reinforcing functions. Such hybrid systems should combine the high absorption capacity of cellulose components with the mechanical strengthening effect of synthetic polymers. This approach allows to achieve a complex effect, in which one component provides technological stability of the mixture at the production stage, and the other increases the operational reliability and durability of the pavement. This approach is of particular relevance when using industrial and secondary materials as raw materials, which allows not only to obtain a product with desired properties, but also to solve important economic and environmental problems. It was this approach that formed the basis for the development of a composite stabilizing additive, the concept and preliminary studies of which were presented earlier in [20, 21]. Within the framework of this article, the main attention is paid to the problem of optimizing its component composition. The goal is not an empirical selection, but a scientific substantiation of rational ranges of component content using mathematical modeling methods.

Materials and methods of research

The stabilizing additive included four main components, which are locally available and secondary raw materials [22]. As a cellulose fiber that performs the function of a binder absorbent, crushed waste paper of the MS-7B grade was used. The source of synthetic polymer fiber, which forms a spatial reinforcing frame, was non-returnable waste from the production of artificial fur and nonwoven fabrics. To prevent thermo-oxidative aging of bitumen on the surface of fibers and agglomeration of granules during storage, a thermal stabilizer, the antioxidant “Diafen FP” (IPPD), was introduced into the composition. The binder for granulating the dry components was road bitumen of the BND 60/90 grade.

To determine the optimal ratio of components, an experiment plan was implemented, which included the preparation and testing of 16 control compositions of the additive. The following were varied as independent variables (factors): the content of synthetic fiber (x_1), crushed waste paper (x_2), thermal stabilizer (x_3), bitumen (x_4) and the dosage of the final additive in the asphalt mixture (x_5).

The effect of the additive was evaluated by the results of the analysis of the physical and mechanical parameters of the control asphalt mixture SMA-15 according to STB 1033 (Republic of Belarus), the granulometric composition of which is presented in Fig. 1. The mixture was prepared using bitumen BND 90/130 in the amount of 6.6 % over the mass of the mineral part. The following indicators were measured as dependent variables (responses): binder drainage (y) (determined by the classical Schellenberg method), tensile strength at 0 °C (P_r) and compressive strength at 50 °C (P_c). The preparation of samples and the conduct of tests were carried out in accordance with the requirements of the STB 1115 standard.

To establish quantitative relationships between the formulation factors and the properties of asphalt concrete, the method of multiple linear regression was used [23].

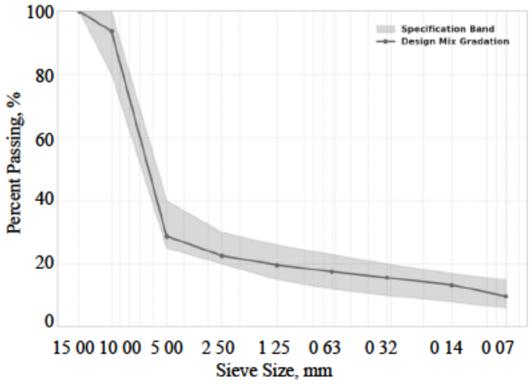

Fig. 1. Aggregate gradation of the control SMA-15 mixture

This statistical approach allows describing the linear relationship between the studied property and several factors. The general form of the model used can be represented by the equation:

$$y = B_o + B_1X_1 + B_2X_2 + \ldots + B_nX_n + \varepsilon. \qquad (1)$$

In this equation, the dependent variable (y) represents the predicted indicator (for example, binder drainage), and the independent variables X_1.. X_n correspond to the formulation factors. The regression coefficients B_1...B_n quantitatively characterize the degree of influence of each factor on the response, B_o is the free term of the equation, and ε denotes the random error of the model.

The calculations were performed in the Python environment using the scikit-learn library. An important methodological aspect when working with compositional data is the prevention of multicollinearity, which arises from the linear relationship between the predictors. Since the sum of the components of the additive is 100 %, the bitumen content (x_4) was excluded from the number of independent variables, since its value is uniquely determined through the other components by the formula:

$$x_4 = 100 - x_1 - x_2 - x_3. \qquad (2)$$

Thus, variables x_1, x_2, x_3 and x_5 were used as predictors in the models. The adequacy and predictive ability of the obtained regression equations were evaluated by generally accepted statistical metrics, namely by the coefficient of determination (R^2) and the root mean square error (*RMSE*).

Results and their discussion

The results of physical and mechanical tests of 16 experimental compositions of asphalt mixture modified with the developed additive are summarized in Table 1.

Table 1

Physical and mechanical properties of asphalt concrete mixture depending on the composition and content of additives

No	Content of the component in the supplement, %				Content of additive in the mixture, % of the mineral part	Indicators		
	Synthetic polymer waste	Shredded waste paper	Heat stabilizer (Diafpen FP)	Bitumen, (BND 60/90)		Binder drainage, %	Tensile strength at 0 °C, MPa	Compressive strength at 50 °C, MPa
1	59	20	9	12	0,1	0,32	2,14	0,92
2	37	37	12	14	0,1	0,29	2,01	0,88
3	31	60	3	6	0,2	0,14	1,98	0,88
4	46	40	6	8	0,2	0,26	2,08	0,9
5	66	10	12	12	0,3	0,34	2,23	0,99
6	20	63	3	14	0,3	0,13	2,12	0,93
7	40	48	6	6	0,4	0,14	2,21	0,99
8	44	39	9	8	0,4	0,15	2,2	0,97
9	18	61	9	12	0,5	0,11	2,18	0,94
10	38	36	12	14	0,5	0,16	2,23	0,98
11	69	22	3	6	0,6	0,19	2,43	1,12
12	48	38	6	8	0,6	0,11	2,36	1,02
13	52	33	3	12	0,7	0,16	2,41	1,06
14	40	40	6	14	0,7	0,1	2,39	1,04
15	42	41	9	8	0,8	0,08	2,39	1,08
16	24	58	12	6	0,8	0,07	2,26	1,01

A preliminary qualitative analysis of the data shows the absence of obvious monotonic dependencies between individual formulation factors and the final properties of the mixture. For example, an increase in the content of one component does not lead to an unambiguous increase or decrease in strength characteristics throughout the entire range of compositions. This confirms the complex, multifactorial nature of the system under study and justifies the need to use mathematical modeling methods to identify hidden patterns. This dataset served as an empirical basis for constructing regression models.

Based on the experimental data presented in Table 1, multiple linear regression models were built that describe the dependence of the studied properties of asphalt concrete on the formulation factors.

The model for predicting binder drainage (*y*) has the form:

$$y = 0.0023x_1 - 0.0028x_2 - 0.0051x_3 - \\ - 0.2836x_5 + 0.3467. \tag{3}$$

The coefficient of determination R^2 = 0,928, the root mean square error *RMSE* = 0,028 %.

The model for predicting the tensile strength limit (P_r) has the form:

$$P_r = 0.0065x_1 - 0.0047x_2 + \\ + 0.0085x_3 + 0.2941x_5 + 1.7488. \tag{4}$$

The coefficient of determination R^2 = 0.906, the root mean square error *RMSE* = 0.053 МПа.

The model for predicting the compressive strength limit (P_c) has the form:

$$P_c = 0.0041x_1 - 0.0029x_2 + 0.0067x_3 + \\ + 0.2588x_5 + 0.6877. \tag{5}$$

The coefficient of determination R^2 = 0.909, the root mean square error *RMSE* = 0.032 МПа.

The high values of the coefficient of determination, exceeding 0.9 for all three models, indicate their high predictive ability and adequacy in the studied range of factors. The analysis of the regression coefficients allows us to give a physical interpretation of the influence of each component. In equation (3), the negative signs at the predictors x_2 (waste paper) and x_3 (thermal stabilizer) confirm their stabilizing effect, which is consistent with the theoretical ideas about the absorption capacity of cellulose. The largest absolute value coefficient at the variable x_5 (–0.2836) quantitatively proves that the total dosage of the additive is the dominant factor in reducing binder drainage.

The analysis of equations (4) and (5) reveals the different roles of the fibrous components in the formation of strength characteristics. The positive coefficients at the variable x_1 (synthetic fiber) in both models confirm its reinforcing function, which consists in creating a spatial frame that increases the strength of asphalt concrete. At the same time, the negative coefficients at the variable x_2 (waste paper) indicate that the cellulose fiber, while effectively performing a stabilizing role, does not make a positive contribution to strength, acting as a softer inclusion in the composite structure. Thus, the obtained models are not only a forecasting tool, but also quantitatively confirm the scientific hypothesis about the separation of functions between the components of the developed additive.

To visually demonstrate the predictive ability of the developed models, graphs comparing the experimental and predicted values for each of the studied properties were plotted (Fig. 2). On these graphs, the experimentally measured values are plotted on the *x-axis*, while the values calculated using equations (3–5) are plotted on the *y-axis*. The diagonal line represents an ideal coincidence between the prediction and the experiment.

As can be seen from the presented figure, for all three models, the experimental points are tightly grouped along the line of ideal coincidence. This arrangement of points is a graphical confirmation of the high values of the coefficient of determination (R^2 > 0.9) and indicates a low prediction error. This allows us to conclude that the developed models are adequate and can be used as a reliable tool for solving the optimization problem.

The process of optimizing the composition consisted in finding such a combination of formulation factors that would simultaneously satisfy the system of given criteria. The value of binder drainage, which should not exceed 0.15 %, was taken as the main limiting criterion. An additional limitation was the tensile strength limit, which should be in the range from 1.5 to 3.5 MPa. The objective function of the optimization was to maximize the compressive strength limit at 50 °C, which provides increased resistance to plastic deformation.

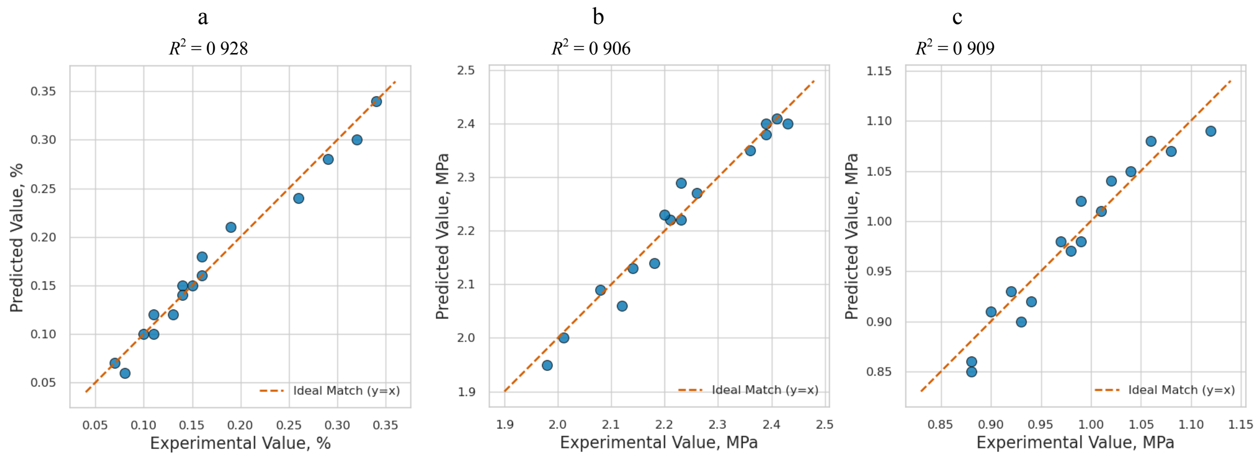

Fig. 2. Comparison of experimental and predicted values for:
a – the binder drainage model (y); b – the tensile strength model (P_r); c – the compressive strength model (P_c)

The use of the obtained regression models (3–5) made it possible to move from the analysis of discrete experimental points to the study of a continuous response surface and to solve the optimization problem analytically. The process of finding the optimal composition was divided into two stages.

At the first stage, using equation (3), the region of admissible solutions was determined. For this, the equation was transformed into an inequality that determines the main limitation on binder drainage:

$$0.0023x_1 - 0.0028x_2 - 0.0051x_3 - \\ - 0.2836x_5 + 0.3467 \le 0.15. \quad (6)$$

An analysis of this inequality allows us to draw key conclusions about the direction of optimization. To fulfill it, it is necessary to increase the values of the variables with negative coefficients, namely the content of waste paper (x_2), thermal stabilizer (x_3) and the total dosage of the additive (x_5). On the contrary, an increase in the content of synthetic fiber (x_1), which has a positive coefficient, complicates the fulfillment of this condition.

To visualize this dependence, a response surface was constructed for binder drainage depending on the content of two key fibrous components (x_1 and x_2) with fixed values of the other factors at a level close to the optimal one (Fig. 3). The red line on the graph indicates the boundary corresponding to the criterion y = 0.15 %. The area to the left of this line represents the desired region of admissible solutions, within which a further search for the optimum in terms of strength characteristics was carried out.

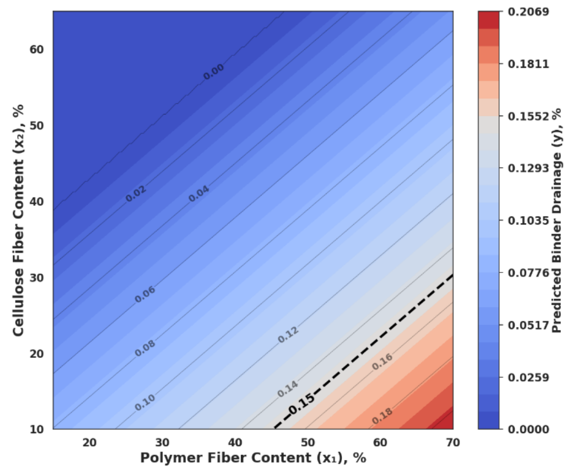

Fig. 3. Response surface for binder drainage (y) as a function of fiber components content (at x_3 = 9 %, x_5 = 0.8 %)

At the second stage, within this found region of admissible solutions, a search was made for the point at which the function of the compressive strength limit P_c (equation 5) reaches its maximum, with the simultaneous observance of the limitation for the function of the tensile strength limit P_r (equation 4). An analysis of equation (5) shows that to maximize strength, it is necessary to increase the content of synthetic fiber (x_1), thermal stabilizer (x_3) and dosage (x_5), but at the same time reduce the content of waste paper (x_2).

A joint analysis of these requirements reveals a key technological contradiction. To minimize binder drainage, a high content of waste paper (x_2)

is required, while to maximize strength, it is necessary to reduce it. This means that there is no solution in which all indicators reach an extremum, and the task is reduced to finding a balanced compromise. To find it, a series of computational experiments was carried out. In the course of these experiments, the dosage of the additive (x_5) was fixed at high, but technologically justified levels (0.6–0.8 %), since it has a positive effect on all target indicators. Further, by varying the content of x_1, x_2 and x_3 in their experimental ranges, with the help of models (3–5), the predicted response values were calculated. From the obtained array of solutions, those that satisfied all the restrictions were selected. Among them was the solution that provides the maximum value of P_c.

This numerical search confirmed that the region of optimal solutions is localized in the region characterized by a content of crushed waste paper (x_2) of about 40 % and higher, a thermal stabilizer (x_3) in the range from 6 to 9 % and a synthetic fiber (x_1) of about 40 %.

For an analytical confirmation of the found optimal region and verification of the predictive ability of the models, a control calculation was performed. For this, a composition was selected that is in the center of the previously determined region: the content of synthetic fiber x_1 = 42 %, crushed waste paper x_2 = 41 %, thermal stabilizer x_3 = 9 % with a dosage of the additive in the mixture x_5 = 0.8 %. Substituting these values into equations (3), (4) and (5) gives the following predicted values. The predicted binder drainage is $y = 0.06$ %. The predicted tensile strength limit is P_r = 2.14 MPa, and the predicted compressive strength limit is P_c = 1.01 MPa.

The obtained calculated values fully satisfy the given optimization criteria. A comparison of these values with the experimental data for the composition No. 15, which is closest in formulation (y = 0.08 %, P_r = 2.39 MPa, P_c = 1.08 MPa), demonstrates good convergence. This further confirms the adequacy of the developed models and the correctness of determining the optimal ranges of component content.

It should be noted that this study has a number of methodological limitations. Firstly, the work is of a laboratory nature, and the findings require confirmation in the course of pilot-industrial tests. Secondly, the applied method of multiple linear regression assumes a linear nature of the dependencies, while the real physical and mechanical processes in a wider range of factors may have a non-linear character. Thirdly, the work was focused on key physical and mechanical indicators, while such an important characteristic as fatigue life was not included in the scope of this study. These limitations, however, do not diminish the value of the findings, but determine the directions for further research.

CONCLUSIONS

The conducted research allows us to draw the following conclusions.

1. The technical feasibility and practical feasibility of creating an effective composite stabilizing additive for stone mastic asphalt based on available secondary raw materials, namely cellulose fiber from waste paper and technogenic polymer fiber from industrial waste, has been confirmed.

2. The method of multiple regression analysis has established itself as a powerful and effective scientific tool for solving multifactorial optimization problems in construction materials science. The constructed mathematical models with high accuracy ($R^2 > 0.9$) adequately describe the dependence of the key properties of asphalt concrete on the additive's formulation, which allows moving from empirical selection to an analytical search for optimal solutions.

3. On the basis of mathematical modeling and solving a multi-criteria optimization problem, the optimal component composition of the stabilizing additive was scientifically substantiated and determined, which ensures the fulfillment of standard requirements: cellulose fiber (39–48 %), synthetic polymer fiber (38–47 %), thermal stabilizer (6–9 %), bitumen (8–12 %).

4. The developed additive, protected by a patent [22], is recommended for use in asphalt mixtures with a high binder content in the amount of 0.3–0.8 % by weight of the mineral part. Its implementation in the practice of road construction provides a twofold economic effect. The direct effect is to replace expensive imported raw materials with available industrial waste. The indirect, long-term effect is associated with a potential increase in the service life of the road surface by improving its strength characteristics, which leads

to a decrease in repair and maintenance costs. At the same time, its use contributes to the solution of the environmental problem of utilization of industrial waste.

5. As promising areas for further research, it is necessary to highlight the conduct of pilot-industrial tests of the developed additive with the construction of experimental sections and the subsequent monitoring of their operational condition. Of scientific interest is also the expansion of the nomenclature of the studied operational characteristics, in particular, the assessment of fatigue life, as well as the use of more complex non-linear models for a more accurate description of the "composition-property" system.

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