The Simpex-Lattice Method Application to Optimize the Design of Soil-Slag-Fly Ash Mixtures

Mateus Henrique R. Rodrigues, Leonardo G. Pedroti, Taciano O. da Silva, Heraldo N. Pitanga, Klaus Henrique de P. Rodrigues, and Emerson C. Lopes

Abstract Ladle furnace slags and fly ashes may be utilized as soil stabilizers in road construction as an option to reuse these by-products. However, there is no method grounded on experimental design to optimize the dosage of those by-products in mixtures with soil. This study applied the Simplex-Lattice method to perform the experimental design to optimize the design of soil-slag-fly ash mixtures. The soil was geomechanically characterized and the by-products were subjected to scanning electronic microscopy (SEM), X-ray diffraction (XRD), pozzolanic activity, and specific surface area analysis. The experimental mixtures were submitted to an unconfined compressive strength test and the results led to a response surface and a mathematical model that described the interaction between the components and allowed the mixture design optimization. This study highlights the potential of the Simplex-Lattice method to optimize soil-slag-fly ash mixtures and the technical suitability of utilizing those by-products as soil stabilizers.

Keywords Steel slag · Fly ash · Simplex-Lattice · Soil stabilization

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Introduction

The steelmaking industry in Brazil is responsible for producing around 35.4 million tons of steel annually; therefore, it is responsible for generating approximately 20 million tons of waste per year. From this total, 27% are classified as steel slag and 6% as fines (including fly ashes) [1]. This considerable volume of waste makes the by-products an undesirable, but inevitable, environmental liability, emphasizing the necessity to find alternatives for their utilization rather than just disposal in nature [2].

These by-products have been successfully applied on the mortars [3], cement [4], and asphalt concrete production [5]. In highway engineering, these materials have shown promising results when used as chemical soil stabilizer agents [6, 7]. The stabilizing potential of those by-products can be optimized when combined with other steelmaking by-products, which is the case of the combined application of ladle furnace slag (LFS) and fly ashes (FA) [8] .

Fly ashes are defined as an artificial pozzolan that, by itself, has few or no agglomeration properties, but when in contact with water, can react with calcium hydroxides creating binding compounds [9]. LFS is a material resulting from secondary steel refining, presenting low hydraulic reactivity, but shows great potential as a chemical agent in soil stabilization applications [6]. Research involving LFS, FA, and other by-products in soil stabilization applications have been carried out using empirical methods based on professional experience to design the mixtures with soil [10]. However, the lack of a consolidated methodology that allows an optimized design of mixtures composed of these by-products and soil, makes it difficult to apply these materials for large-scale production. In order to suppress this difficulty, some statistical design methods have been studied for this purpose, such as the Simplex-Lattice method, which is a promising method that has been successfully used in the optimized design of ceramic compounds [11], mortars [12], and other product varieties.

The Simplex-Lattice method can be described as an ordered system consisting of a uniformly spaced points arrangement, that must be tested, and which results are used to fit a regression model. An advantage of applying this method while designing mixtures is to reduce the number of trials required to get a regression model to predict the mixtures response in function of mix ratio components [13].

The present paper evaluates the Simplex-Lattice method technical applicability on the optimized design of Soil-Ladle Furnace Slag-Fly Ash (SLF) mixtures, aiming to maximize the unconfined compressive strength of these mixtures. To study the mixtures responses and to evaluate the potential of the application of these by-products as a chemical stabilizer in soil stabilization applications, it was also proposed performing the physical, mineralogical, and chemical characterization of the raw materials.

Materials and Methods

Materials

The soil sample used in this study was collected in Viçosa, Minas Gerais State, Brazil, submitted to air-drying, and prepared to perform the laboratory tests in accordance with NBR 6457 [14].

The LFS sample was obtained from a steelmaking company located in Jeceaba, Minas Gerais State, Brazil. The material sampling was carried out in accordance with NBR 10007 [15]. After transporting the material to the Civil Engineering Laboratory at the Federal University of Viçosa, the material was air-dried, milled, and submitted to a sieving process to retain the particles larger than 0.6 mm (sieve nº 30).

The FA used in this study was obtained from a company responsible for processing and commercialize pozzolanic fly ash from coal burning, located in Capivari de Baixo, Santa Catarina State, Brazil. The material is classified as class-C fly ash and meets the pozzolanic requirements prescribed in technical standard NBR 12653 [16].

Characterization of Raw Materials

Soil sample was submitted to characterization laboratory tests to determine: (i) the particle size distribution [17]; (ii) specific gravity [18]; and (iii) Atterberg Limits and Plasticity Index [19, 20]. Samples of LFS and FA were submitted to laboratory tests to determine the specific gravity [21], the finesses by sieving [22], and the specific surface area by Brunauer, Emmett, Teller (BET) method. The pozzolanic activity test performed on steel slag and fly ash samples were carried out following the procedures proposed by Lúxan et al. [23].

The mineralogical characterization of soil, ladle furnace steel slag and fly ash, were carried out by means of XRD diffraction test, utilizing Brunker D-8 Discover diffractometer (CuKα radiation, 40 kV, 30 mA, $\lambda = 1.5418$ Å, θ–2θ angles, 5º a 80º range, 0.02°/step, 1 s/step). Scanning electron microscopy (SEM) analysis was also performed on LFS and FA samples, utilizing JOEL JSM-6010LA equipment, utilizing sputter coated specimens to prevent charging in the SEM.

Experimental Design of Mixtures

The method chosen to design the experimental mixtures was the Simplex-Centroid method. The experimental mixtures were composed of three components (soil, LFS, and FA), therefore, the total experimental mixtures to be tested in this experimental program is given by (2^q–1), where "q" corresponds to the number of components on the mixture [24], totalizing 7 mixtures. Additionally, it was proposed that the

Fig. 1 Simplex-Centroid triangular diagram and testing mixtures identification

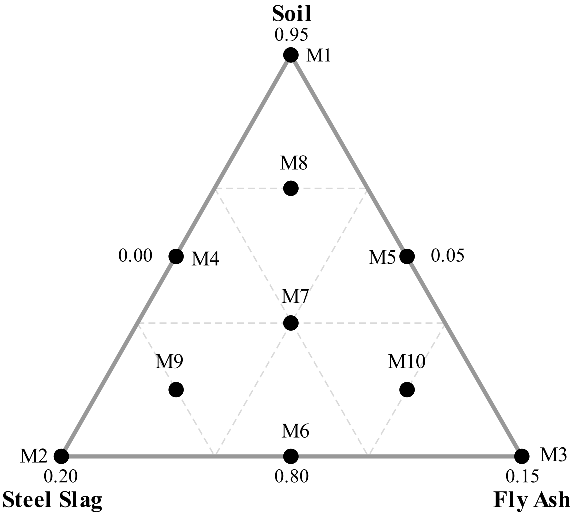

Table 1 Component contents of the experimental mixtures (dry mass composition)

Material	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10
Soil (%)	95.0	87.5	80.0	80.0	80.0	87.5	85.0	82.5	82.5	90.0
LFS (%)	5.0	12.5	20.0	12.5	5.0	5.0	10.0	7.5	15.0	7.5
Fly Ash (%)	0.0	0.0	0.0	7.5	15.0	7.5	5.0	10.0	2.5	2.5

3 intermediate mixtures were to be tested, as shown in Fig. 1. The maximum and minimum limits that all components can assume in the mix proportion were defined based on values verified in the technical literature [25], being defined that the mixtures would be composed by 5–20% of LFS and 0–15% of FA. The composition of each experimental mixture is presented on Table 1.

Testing Methods

The natural soil and all the experimental mixtures were submitted to a compaction test, in accordance with NBR 7182 [26], to define the maximum dry unit weight and the optimum moisture content. Three specimens of each experimental mixture and three specimens of natural soil were submitted to unconfined compressive strength (UCS) test in accordance with NBR 12770 [27], considering the Standard Proctor compaction energy and 7 days curing period. The UCS of each mixture was determined from the mean value obtained from the three tested specimens. The UCS of the natural soil was determined following the same procedure adopted for the experimental mixtures.

Table 2 Geotechnical characterization of soil

Geotechnical parameter	Result	Geotechnical parameter	Result
Clay (%) ($\Phi \leq 0.002$ mm)	5	Bulk Specific Gravity (g/cm^3)	2.657
Silt (%) (0.002 mm < $\Phi \leq 0.06$ mm)	24	Liquidity Limity (LL) (%)	36
Fine sand (%) (0.06 mm < $\Phi \leq$ 0.2 mm)	13	Plasticity Limit (PL) (%)	18
Medium Sand (%) (0.2 mm < $\Phi \leq$ 0.6 mm)	40	Plasticity Index (PI) (%)	18
Gravel Sand (%) (0.6 mm < $\Phi \leq$ 2 mm)	15	USCS Classification	SC
Gravel (%) ($\Phi > 2.0$ mm)	3	TRB Classification	A-2-6

The UCS result for each mixture was uploaded in Minitab® software to generate the mathematical model that describes the interaction between components and their impact on the product mechanical behavior. To the statistical analysis it was setup a confidence level of 95%.

Results and Discussion

Geotechnical Characterization of Soil

Table 2 presents the results from the geotechnical characterization of soil and the soil classification according to the Unified System of Classification of soils (USCS) and Transportation Research Board (TRB). The soil can be classified as a clayed sand soil according to USCS and as A-2-6 soil according to (TRB). The soil particle size distribution is shown in Fig. 2.

Mineralogical Characterization

Figure 3a and b show, respectively, the ladle furnace steel slag and the fly ash SEM images. From the SEM images, it is noted that LFS has very irregular shaped particles, while the fly ash is composed of particles fine-grained and spherical in shape. Irregularly shaped particles have a lower specific surface area compared to spherical particles. For materials that present cementitious properties, it is desirable that these materials show high specific surface area since the amount of chemical reactions tends to be proportional to this factor.

Figures 4 and 5 presents the major mineralogic phases identified in the ladle furnace slag and in the fly ash samples, respectively. The major phases identified in the ladle steel slag were the portlandite, olivine, calcite, dolomite, brucite, artinite,

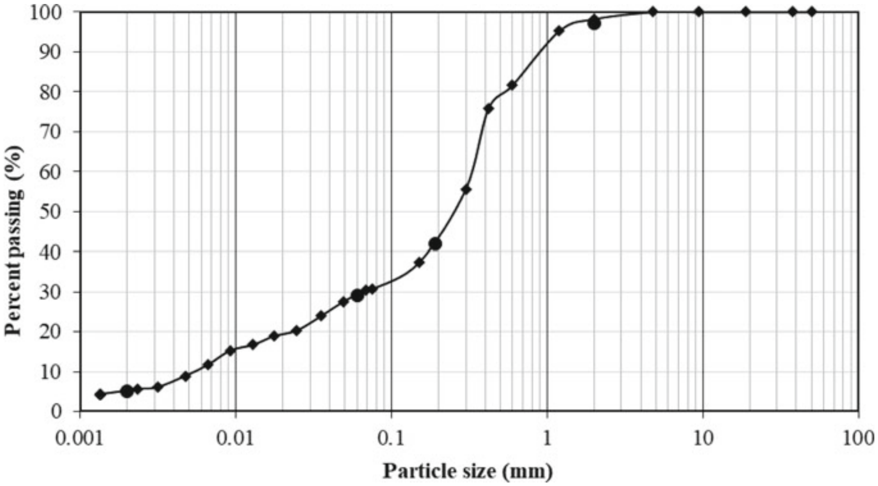

Fig. 2 Soil grain size distribution

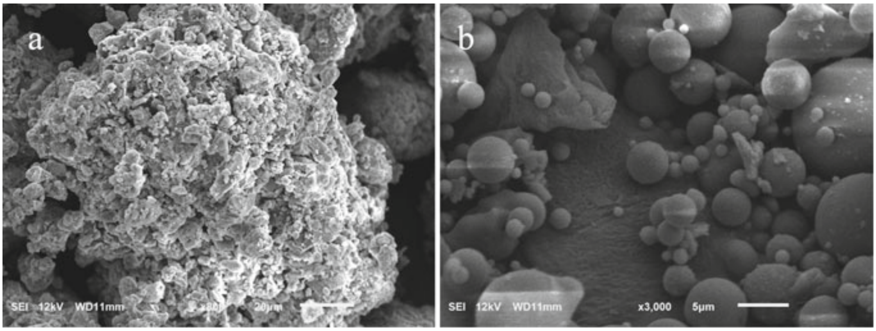

Fig. 3 Ladle furnace steel slag **a** SEM image and fly ash **b** SEM image

and larnite, while in the fly ash sample were identified the mullite, wollastonite, quartz, lime, calcite, albite, anhydrite. The peaks on the XRD patterns indicate the amount of the mineralogic phases in the materials composition. Both the mineralogic phases and the amount of these phases in the materials compositions were the same verified in some studies approaching the same type of materials, except for the olivine in the LFS, and for the mullite in the FA, which has shown a larger amount than what is observed in the technical literature consulted [6–8, 28].

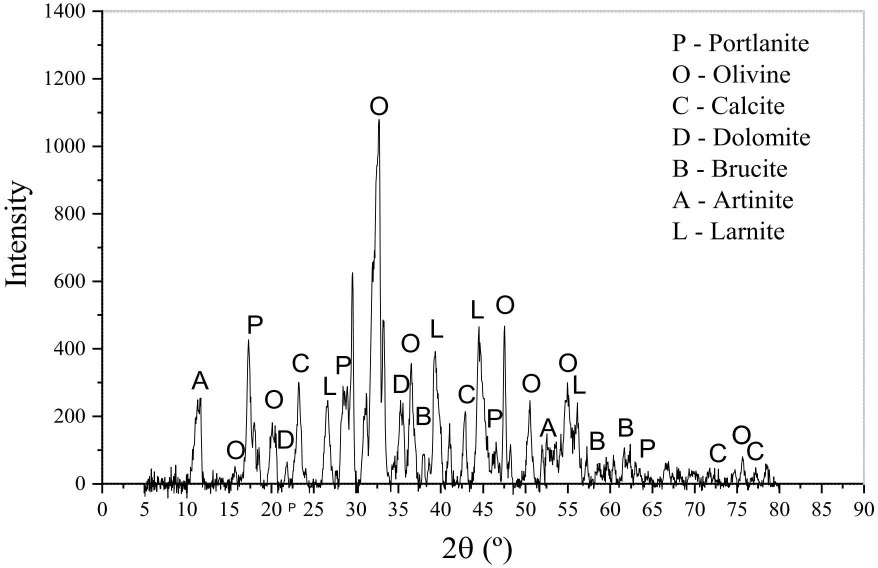

Fig. 4 Results of the XRD analysis of the ladle furnace steel slag sample

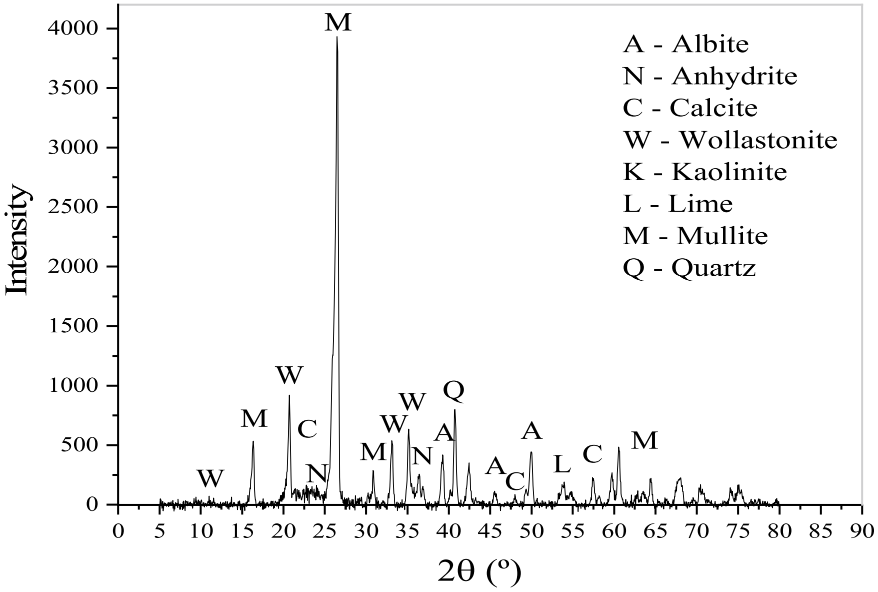

Fig. 5 Results of the XRD analysis of the fly ash sample

Table 3 Physical and chemical characterization of ladle furnace steel slag and fly ash samples

Properties	LFS	Fly Ash
Finesses index (%)	55.8	23.71
Blaine Specific Surface Area (cm^2/g)	1906.4	1788.24
Specific Gravity (g/cm^3) -	2.91	2.08
Pozzolanic Activity (Lúxan et al. 1989)	Low	Medium

Chemical and Physical Characterization of Raw Materials

The results from the characterization tests performed on the by-products are shown in Table 3. The LFS has larger specific gravity compared to fly ash, which is in accordance with usual values for the specific gravity of these materials [29]. Both materials have shown a high specific surface area, indicating a favorable condition to occur hydration reactions. The finesses index for both materials indicates that the fly ash has a larger amount of fines compared to the ladle furnace slag. The fly ash response to the pozzolanic activity test performed indicates that this material has medium pozzolanic activity, while the ladle furnace slag sample presented low pozzolanic activity. Even though those materials have not shown good pozzolanic activity, the combined application of those materials may be interesting; the fly ash has a higher amount of artificial pozzolanic components and the steel slag has higher contents of cementitious compounds, which when combined, favors hydration reactions [25].

Geotechnical Characterization of Experimental Mixtures and Natural Soil

Figure 6 shows the maximum dry unit weight and the optimum moisture content for each experimental mixture and for the natural soil submitted to the compaction test. From Fig. 6, the variation in the maximum dry unit weight and moisture content between the mixtures can be observed, showing that the by-products addition has increased the maximum dry unit weight and the optimum moisture content of the mixtures when compared to the natural soil. The soil maximum dry unit weight was 1.717 g/cm^3 at 15.1% of water content. The higher maximum dry unit weight was observed for the mixture containing 20% of ladle steel slag on its composition. Also, an increase in the optimum moisture content proportional to the amount of by-product in the mixture was observed. This behavior is assigned due to the amount of fines in the mixture increase, which increases the mixture specific surface area and requires higher amount of water to hydrate the cementitious compounds added to the mixtures [16].

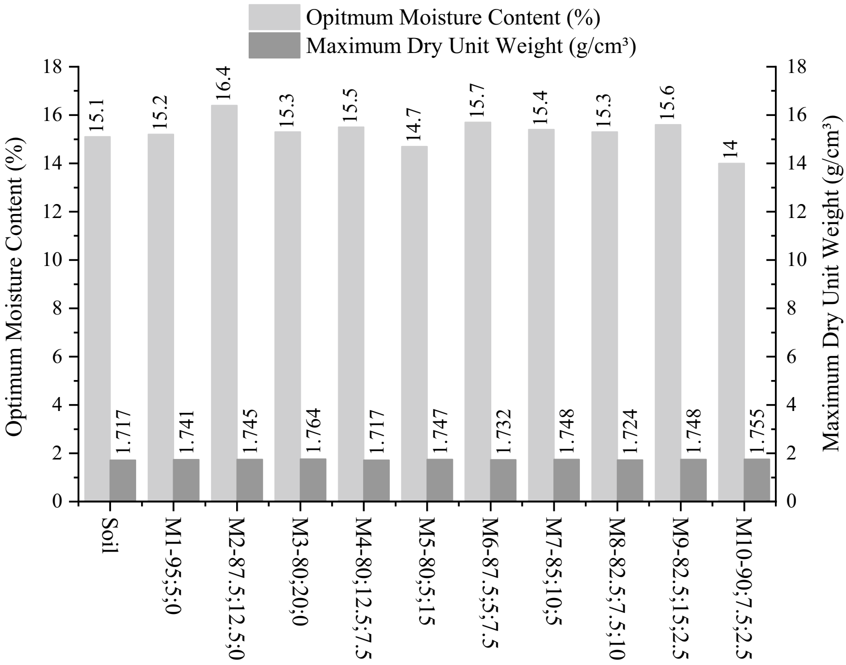

Fig. 6 Experimental mixtures optimum water content and maximum dry unit weight

Unconfined Compressive Strength Tests

The results from the UCS tests performed are shown in Fig. 7. The addition of steelmaking by-products in the mixtures has improved the compressive strength of the natural soil, by 14 to 62%. The experimental mixtures that shown the highest UCSs were mixtures M3, M4, M5, and M7, with a maximum UCS of 166 kPa corresponding to the M5 mixture. This value represents a significant increase of 62% in the unconfined compressive strength of natural soil, suggesting a baseline for optimization of materials combinations.

The verified gain in soils compressive strength can be assumed as a consequence of cementitious and hydration reactions that originate cemented components along the curing time considered. This hypothesis is taken as an explanation when considering the XRD analyses indicating the presence of minerals such as larnite, mayenite, and wollastonite in the materials structure desirable hydraulic properties [6, 10].

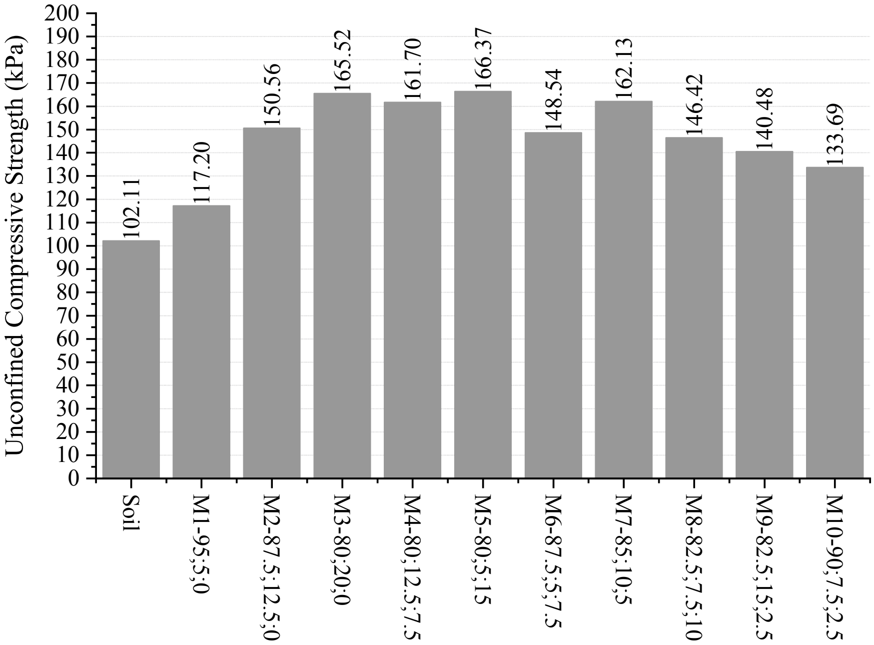

Fig. 7 Unconfined Compressive Strength tests results

Simplex-Lattice Method Analysis

The UCS results from each experimental mixture were assessed in Matlab 2018® software to obtain the triangular response surface shown in Fig. 8, from which can be observed the resistance intervals as a function of the proportion of each component in the mixture.

As the mixtures were composed of three materials, the mathematical model proposed to describe the UCS behavior of the mixtures has the structure presented in Eq. 1 [25], where "Y" represents the unconfined compressive strength, "β_x" the regression coefficients, and "x_i" the amount of each component in the mixture.

$$Y(x_1x_2x_3) = \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{23}x_2x_3 + \beta_{123}x_1x_2x_3 \tag{1}$$

The most statistically fitted regression model calculated, considering 95% of confidence level, is shown in Eq. 2. In this equation, the UCS is expressed as a function of the proportion of soil (S), ladle furnace slag (L), and Fly ash (F) in the mixture composition.

$$UCS(kPa) = 109.6\,S + 369.6\,L + 382.1F \tag{2}$$

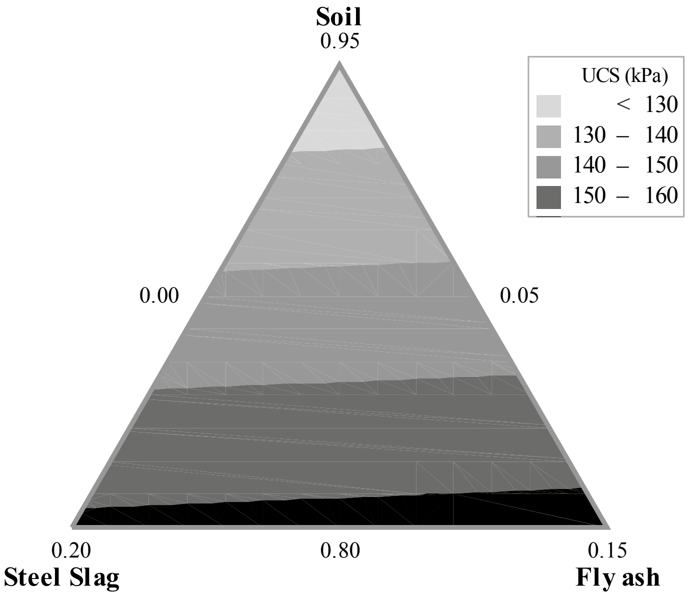

Fig. 8 Response surface for UCS as a function of material content

From the regression model coefficients presented in Eq. 2, can be inferred that the LFS and the FA addition in the mixture composition has a positive influence on the mixture's unconfined compressive strength. The coefficients that represent the interaction between the components as shown in Eq. 1 (β_{12}, β_{13}, β_{23}, β_{123}) did not present statistical relevance and have been removed from the regression model. The regression model presented in Eq. 2 resulted in R^2 equals to 71.72%.

From the mathematical model presented in Eq. 2, it was possible to optimize the mix design through the statistical tool "desirability" available from the Minitab® software to maximize the UCS. This approach was carried out with a set UCS target value of 170 kPa. As a result of this optimizing procedure, the Minitab ® software returned the mixture composed of 80% of soil, 5% of LFS, and 15% of FA as the optimal mixture with a desirability value equal to 0.962, and a maximum UCS of 166.4 kPa.

Conclusion

The Simplex-Lattice method is a powerful tool to perform the experimental design of mixtures aiming to evaluate the product's responses as a function of the mixture components contents. This method significantly reduces the number of trials required to achieve the balance between the materials ratio in the mixture and their mechanical response. In addition, the Simplex-Lattice method can establish a response surface consistent with the testing results, allowing the possibility to define different proportions that are able to reach the same range of UCS, and making suitable the optimized design of mixtures.

The unconfined compressive strength of the natural soil has increased up to 62% by applying different materials proportions in the mixtures. The observed behavior is attributed to pozzolanic and cementitious reactions between the steelmaking by-products and the soil, since the mineralogical characterization of those materials verified the presence of mineralogic phases that indicates high cementitious potential, such as larnite, mayenite and wollastonite, and belite.

From the significant improvement on soil performance under this loading condition, it is verified the technical suitability of the application of ladle furnace slag and fly ash as soil stabilizer agents, consolidating an interesting alternative to reuse a large amount of those by-products.

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