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Modelling of cement raw material compositional indices with direct sequential cosimulation

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ABSTRACT

Spatial distribution of cement raw material compositional indices is a precondition of conducting quarry stope layouts. These indices are calculated from chemical components, such as SiO_2, Al_2O_3, Fe_2O_3, CaO and MgO, and the most important are LSF (lime saturation factor), SIM (silica modulus), ALM (alumina modulus) and CS (lime silica ratio). Geostatistical images of the grades are more useful in this respect, as they reflect different representations of the reality and show the spatial distribution more accurately. This paper presents the construction of sets of simulated images of the chemical components SiO_2, Al_2O_3, Fe_2O_3, CaO and MgO as primary variables, using the direct sequential simulation (DSS) and cosimulation (CoDSS) algorithms. For the joint simulation, a novel methodology uses principal components (PC) as secondary variables. Finally, the simulated images are combined algebraically in order to estimate local distribution functions of the compositional indices (LSF, ALM, SIM and CS), showing whether the local probability of each index is within the optimal interval.

1. Introduction

Cement, the basic ingredient of concrete, is a closely controlled chemical combination of calcium, silicon, aluminium, iron and small amounts of other ingredients to which gypsum is added in the final grinding process to regulate the setting time of the concrete. Lime and silica make up about 85% of the mass. Common among the materials used in its manufacture are limestone, shells, and chalk or marl combined with shale, clay, slate or blast furnace slag, silica sand, and iron ore. Each step in the manufacture of cement, such as quarry extraction of raw materials, is checked by frequent chemical and physical tests in plant laboratories. The final product is also analyzed and tested to ensure it complies with specifications (IPQ, 2001). Spatial distribution of cement raw material compositional indices is a precondition of conducting quarry stope layouts. These indices are calculated from weighted percentages of chemical components, such as SiO_2, Al_2O_3, Fe_2O_3, CaO and MgO, and the most important are LSF (lime saturation factor), SIM (silica modulus), ALM (alumina modulus) and CS (lime silica ratio).

The LST or lime saturation factor is the ratio between calcium and the weighted sum of the silica, alumina and iron amounts by weight:

$$LSF = \frac{CaO}{2.8SiO_2 + 1.18Al_2O_3 + 0.65Fe_2O_3}. \quad (1)$$

When the raw materials are correctly mixed and under proper burning conditions, no free CaO should be left in the clinker. Theoretically, the LSF should range between 0.66 and 1.02, but is optimal if between 1 and 1.02. Higher values are better as the cement's mechanical resistance is improved, however, the raw materials must be ground more finely and the clinker temperature must be higher, leading to damage to the furnace walls.

The SIM, or silica modulus, also known as the silica ratio, is the second most important index and represents the relationship between the silica and the sum of the alumina and iron grades:

$$SIM = \frac{SiO_2}{Al_2O_3 + Fe_2O_3}. \quad (2)$$

A high SIM raw material produces a clinker with a high grade of silicates, and consequently cement with high mechanical resistance. However, high SIM rates have disadvantages, such as a low percentage of the liquid phase, difficulty in clinkerization and the need for higher temperatures, increasing fuel consumption. However, the advantages of a low SIM are a higher percentage of the liquid phase, facilitating clinkerization, with low burn temperatures, and therefore less energy consumption. SIM values usually range between 2.4 and 2.6.

The ALM or alumina modulus is calculated as the ratio between alumina and iron:

$$ALM = \frac{Al_2O_3}{Fe_2O_3}. \quad (3)$$

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Suitable ALM values range between 1.5 and 1.7.

On the other hand, the ratio between calcium and silica (*CS*) should be higher than 2.0:

$$CS = \frac{CaO}{SiO_2 \geq 2.0.} \quad (4)$$

Finally, the magnesium grade (MgO) should be below 5% weight:

$$MgO < 5\%. \quad (5)$$

Geostatistical techniques in earth sciences are able to produce an average image (estimation) or a set of equiprobable images (simulation) of the spatial distribution of petrophysical or geochemical variables (Matheron et al., 1987; Journel and Alabert, 1988; Srivastava, 1994; Goovaerts, 1997; Deutsch and Journel, 1998). They are often used in evaluation of reserves and mine/quarry exploitation planning (Taboada et al., 1999; Tercan and Özçelik, 2000; Emery and Silva, 2009).

In simulation methods, the intention is not to produce an average image, or the most likely image, of the characteristics of the resource (the objective of any estimation, for example kriging), but a set of realistic images showing extreme behaviours and local and global uncertainty. Each simulated image is a particular realization of a random function, keeping the same spatial distribution, basic statistics (histogram) and spatial variability (variogram or spatial covariance) as the experimental data.

To simulate images of compositional indices, two approaches can be used: generation of images of grades and subsequent calculation of indices, or immediate generation of images treating the indices as random variables. In our paper, we decided to (co)simulate first the five chemical components (SiO_2, Al_2O_3, Fe_2O_3, CaO and MgO), the compositional indices being constructed subsequently. This procedure is mainly justified by the lower spatial continuity of the indices compared with the chemical components, given that they are combined by a math formula and the chemical components are not all highly correlated. On the other hand, all five chemical components show a well-defined spatial structure, as demonstrated by the variograms and corroborated by the stratification orientation visible in the quarry.

Several simulation methods are candidates to generate images of the oxide components, notably sequential simulation. Sequential Gaussian simulation (SGS) and sequential indicator simulation (SIS) were the first versions used (Journel, 1989; Goovaerts, 1997; Deutsch and Journel, 1998). More recently, DSS such as that proposed by Caers (2000) and improved by Soares (2001) became widely used sequential simulation techniques for continuous variables, avoiding transformations to normal score space and facilitating the use of secondary information (Robertson et al., 2006; Emery and Silva, 2009). In the present work, direct sequential simulation and cosimulation were used (DSS and CoDSS).

In multivariable environments, CoDSS are a good candidate to simulate the entire set of variables preserving the intrinsic relationships between variables (as measured by correlation coefficients and variograms). In CoDSS, local mean and variance can be estimated with simple cokriging if all variables are simulated at once (Journel and Huijbregts, 1978; Goulard and Voltz, 1992) or simple collocated cokriging if variables are simulated one at a time (Almeida and Journel, 1994). However, and especially with more than two variables, modelling a coregionalization is a difficult problem that can only be solved by assuming simplifications.

In the present paper, for the joint simulation of chemical components or primary variables (SiO_2, Al_2O_3, Fe_2O_3, CaO and MgO), a novel methodology uses the principal components (PC) of principal component analysis (PCA) as secondary variables. Finally, the simulated images are combined algebraically in order to estimate local distribution functions of the compositional/quality indices (LSF, ALM, SIM and CS), showing whether the local probability of each index is within the optimal interval.

A case study on the Outão cement plant illustrates the proposed methodology. Samples were collected at the quarry stopes from an approximately regular mesh of vertical boreholes and chemically analyzed by X-ray fluorescence.

2. Methodology

2.1. Framework

The main goal of the proposed methodology is to produce sets of simulated images of the compositional indices described above and zoning of the most appropriate areas in terms of raw material, in the following steps:

1 Exploratory univariate and bivariate statistical analysis of the chemical components (primary variables) under study: SiO_2, Al_2O_3, Fe_2O_3, CaO and MgO.
2 For the primary variables, application of principal component analysis (PCA) and selection of the principal components (PC) to use as secondary data, usually two or three, that explains most of the variance.
3 Correlation analysis between the selected PC (secondary data) and the chemical components (primary data);
4 Calculation of experimental variograms and fitting of theoretical models for the selected PC and the primary variables.
5 Stochastic simulation of N_s images of each selected PC, using DSS. Each set of N_s simulated images will be considered secondary data in the following stages of this methodology. It is important to note the independence between the PCs, which justifies the use of DSS, not CoDSS.
6 Cosimulation of N_s images of each chemical component (primary data), conditioned to the sample data and sets of simulated images of the PCs (secondary data) with CoDSS.
7 Calculation of N_s images of cement's compositional index (SIM, ALM, LSF and CS) by algebraic combination of the simulated images of the chemical components, according to Eqs. (1)–(4). Locally, the set of N_s values constitutes an estimation of the local histogram of these indices.

The simulated images obtained in step 7) enable the generation of exploitation scenarios and optimal strategies for planning of raw materials mixtures, highlighting global and local uncertainties. Indicator maps and zoning of areas in which the compositional indices (SIM, ALM, LSF, CS and grade of MgO) display values in the optimal intervals are another important issue on the basis of the N_s simulated images of indices.

2.2. Process steps of DSS and CoDSS

To explain the cosimulation of a grid of values with N locations (x_u) we first denote $Z_1(x)$ as the primary random variable and $Z_2(x)$ as the secondary random variable.

The DSS steps are as follows (Soares, 2001):

i) Selection of a random sequence with a single visit to each grid location x_u to be simulated.
ii) At each grid location x_u, simulation of the $z_2^s(x_u)$:
  – Estimation of the local mean and variance of $Z_2(x)$ at grid location x_u, $z_2(x_u)^*$ and $\sigma^2_{z_2}(x_u)^*$ by simple kriging.
  – Local resampling of the histogram of $z_2(x_u)$ using, for instance, a Gaussian transformation (φ_2) of the variable $Z_2(x)$; calculation of $y(x_u)^* = \varphi_2[z_2(x_u)^*]$.
  – Generation of a random number p from the uniform distribution function U defined between [0;1].
  – Generation of the value y^s from the Gaussian distribution $G(y(x_u)^*, \sigma^2_{z_2}(x_u)^*)$: $y^s = G^{-1}(y(x_u)^*, \sigma^2_{z_2}(x_u)^*, p)$.
  – Inverse transformation and generation of the simulated value of the secondary variable $z_2^s(x_u) = \varphi_2^{-1}(y^s)$.
iii) Loop until all N grid locations are simulated.