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**Book of Extended  
Abstracts**

**INTERNATIONAL  
CONFERENCE on Mathematical  
Analysis and Applications in  
Science and Engineering  
ICMA<sup>2</sup>SC'22**

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**Dedication**

In memoriam of Professor J.A. Tenreiro Machado (1957 - 2021), an enthusiastic scientist, respected colleague, generous person, and trustworthy friend. More information [here](#).



Professor J.A. Tenreiro Machado (1957 - 2021)

## Numerical modeling and optimization of self-compacting mortars: central composite design approach with

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### Abstract:

The current work developed Statistical models to reach high-performance self-compacting cement-based mortars for structural purposes. A central composite design approach was employed to describe mortar fresh and hardened properties (mechanical strength) in function of key mortar mixture design parameters. The fitted models allow to model and predict flowability and viscosity properties and find a range where self-compacting behavior existed. Sand to mortar volume ratio exhibited the main effect on flowability and viscosity, with a positive effect, which is explained by decreases in paste volume. As expected, the water to cement volume ratio had the highest effect on both flexure and mechanical strength of mortars.

keywords: Design of experiments;  
response model;

MSC2010: 26A##; 34A##; 93B##.

## 1 Introduction

The design of cement-based materials can be complex since they must meet several current requirements. Even though the selection of the material should try to improve robustness, making the mixture more tolerant to raw material variability, for economic reasons, it depends much on local availability so there is no fixed rule for the amount/type of aggregates, cement, additions and admixtures [1]. Thus, a decisive factor for the design of advanced cementitious materials, such as SCC, is the clear understanding of the effect of each constituent raw material and their interactions on final product properties [2]. Besides, the design and optimization of such mixtures need intensive laboratory testing, particularly if new and unconventional supplementary cementitious materials or aggregates are incorporated [3]. Therefore, a more scientific and multi-scale approach to mix-design is needed, in which key mixture design variables can explain the composite properties. DOE allows to mathematically model the influence of mixture parameters on relevant composite properties and their interactions [4], to allow an appropriate adjustment for individual constraining, as raw materials or "in situ" conditions, and come up with an optimal mixture for specifically defined requirements, including cost and sustainability indicators, in a reduced time [5], [6], [7], [8]. In the current work statistical analysis of data, model fitting, validation and optimization from data available in the literature at [9] concerning a full central composite design employed to optimize high-performance self-compacting cement-based mortars were performed. The objective of the central composite design (CCD) developed was to fit a model to mathematically describe the fresh (flowability and viscosity) and hardened (flexural and compressive strength) state properties of high-performance self-compacting cement-based mortars.

## 2 Central composite design

Maia (2021) (Maia 2021) performed a wide experimental programme in high performance self-compacting mortars, by means of a full CCD  $2^5$ . In total, 64 mortar mix compositions were done that corresponded to a full factorial design  $2^5$  augmented by 10 axial runs plus 8 central runs, resulting in a CCD with 50 mortar trial mix composition. The CCD complied five independent variables (factors): (i)  $V_w / V_c$  - water to cement volume ratio; (ii)  $Sp/p$  - superplasticizer to powder mass ratio; (iii)  $V_w/V_p$  - water to powder volume ratio; (iv)  $V_s/V_m$  - sand to mortar volume ratio; (v)  $V_{fs}/V_s$  - fine sand to total sand volume ratio. The effect of each key factor was evaluated at five levels  $-\alpha, -1, 0, +1, +\alpha$ , as shown in Table 1. In order to make the design rotatable, the value of  $\alpha$  was taken equal to  $n_F^{1/4}$ , where  $n_F$  is the number of points in the factorial part of the design. In the current study, this corresponds to taking an equal to 2.3784. Four dependent variables, i.e., response variables, were considered: (i) slump-flow diameter (D-flow); (ii) the time in the V-funnel (T-funnel); (iii) flexural strength, at 24 hours, determined by the three-point loading method (F,24h); (iv) uniaxial compressive strength at 24 hours (Rc,24h) (Maia 2021).

Table 1 - Correspondence between coded values and actual values of design variables.

| Design Variables  | -2.3784 | -1    | 0     | +1    | +2.3784 |
|-------------------|---------|-------|-------|-------|---------|
| $X_1: V_w/V_c$    | 0.682   | 0.805 | 0.895 | 0.894 | 1.108   |
| $X_2: Sp/p$       | 0.019   | 0.022 | 0.024 | 0.025 | 0.029   |
| $X_3: V_w/V_p$    | 0.434   | 0.513 | 0.570 | 0.627 | 0.706   |
| $X_4: V_s/V_m$    | 0.366   | 0.432 | 0.480 | 0.528 | 0.594   |
| $X_5: V_{fs}/V_s$ | 0.043   | 0.250 | 0.400 | 0.550 | 0.757   |

## 3 Response models

The statistical procedure to obtain regression models to describe the response variables in terms of design variables consisted in: (i) Fitting a second-order polynomial model using regression analysis and ANOVA including the removal of non-significant terms in the model (p-value >0.05) and using backward method to eliminate non-significant terms in the regression model;

(ii) Model adequacy checking and diagnosis (plot analysis, Kolmogorov–Smirnov, Shapiro-Wilk, Durbin-Watson, Cook's distances); (iii) Evaluation of significant individual and interaction effects, among other computations; (iv) Mixtures optimization using desirability function. Design-Expert software was used to assist in: analyses the results for each response variable by examining summary plots of the data, fitting a model using regression analysis and ANOVA, validating the model by examining the residuals for trends and outliers, leverage points, autocorrelation and violation of statistical assumptions, in general, and interpreting the model graphically. The central composite design adopted allows for the estimation of a full quadratic model as presented in Equation Eq. 1.

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i < j} \sum \beta_{ij} x_i x_j + \varepsilon \quad \text{Eq. 1}$$

where  $y$  represents the response variable;  $x_i$  correspond to the design variables considered; the letter  $\beta$  is used for model parameters ( $\beta_0$  is the independent term,  $\beta_i$  represents the linear effect of  $x$ ,  $\beta_{ii}$  represents the quadratic effect of  $x_i$  and  $\beta_{ij}$  represents the linear-by-linear interaction between  $x_i$  and  $x_j$ ); and  $\varepsilon$  is the fitting error. The model parameters ( $\beta_0$ ,  $\beta_i$ ,  $\beta_{ij}$ ) can be estimated by means of a multilinear regression analysis. In the course of the analysis, it may happen that some of the terms in Eq. (1) may not be significant. The final equations in terms of coded factors are presented in Table 2. A variable transformation of the form  $1/y$  was used in order to stabilize the Tfunnel response variance and improve the resulting model, which is in accordance with previous studies [6], [10]. From the coded equation can be identified the relative impact of the factors by comparing the factor coefficients. Higher values indicate higher influence of the design variable in the response. For each model, the three most significant parameters are typed bold and the most significant term is also underlined. A positive coefficient means that the response (or transformed response) variable will increase if the given mixture parameter increases and vice-versa.

Table 2 – Fitted models (design variables in coded values).

| Model Terms                  | D-flow (mm)          | 1/T-funnel (s)        | F,24h                 | Rc,24h              |
|------------------------------|----------------------|-----------------------|-----------------------|---------------------|
| Independent                  | 343.75               | 0.0688                | 11.43                 | 60.65               |
| Vw/Vc                        | 8.92                 | <b>0.0115</b>         | <b><u>-0.4053</u></b> | <b><u>-6.17</u></b> |
| Sp/p                         | 4.58                 | 0.0050                | NS                    | NS                  |
| Vw/Vp                        | <b>19.42</b>         | <b>0.0245</b>         | <b>-0.2610</b>        | <b>-1.19</b>        |
| Vs/Vm                        | <b><u>-34.92</u></b> | <b><u>-0.0302</u></b> | 0.2608                | 0.2655              |
| Vfs/Vs                       | -1.42                | -0.0016               | NS                    | <b>-1.33</b>        |
| (Vw/Vc) x (Vw/Vp)            | -5.36                | NS                    | NS                    | NS                  |
| (Vw/Vc) x (Sp/p)             | -2.89                | -0.0020               | NS                    | NS                  |
| (Vw/Vc) x (Vs/Vm)            | NS                   | -0.0037               | NS                    | NS                  |
| (Vw/Vp) x (Vs/Vm)            | 3.11                 | -0.0061               | 0.1826                | NS                  |
| (Vw/Vp) x (Vfs/Vs)           | 2.98                 | NS                    | NS                    | NS                  |
| (Sp/p) x (Vfs/Vs)            | 1.89                 | NS                    | NS                    | NS                  |
| (Vs/Vm) x (Vfs/Vs)           | NS                   | NS                    | NS                    | -0.4934             |
| (Vw/Vc) <sup>2</sup>         | <b>-20.67</b>        | -0.0017               | NS                    | 0.5639              |
| (Vw/Vp) <sup>2</sup>         | NS                   | 0.0011                | NS                    | 0.5486              |
| (Vs/Vm) <sup>2</sup>         | NS                   | NS                    | <b>-0.2834</b>        | NS                  |
| (Vfs/Vs) <sup>2</sup>        | NS                   | -0.0014               | NS                    | NS                  |
| Error term ( $\varepsilon$ ) |                      |                       |                       |                     |
| R <sup>2</sup>               | 0.9858               | 0.9922                | 0.6619                | 0.9588              |
| Adj-R <sup>2</sup>           | 0.9802               | 0.9897                | 0.6216                | 0.9519              |

NS: non-significant term. The three most significant parameters are typed **bold** and the most significant term is also underlined.

From regression models presented in Table 1, it can be perceived that Vs/Vm exhibited the strongest effect, a negative effect, on the fresh state properties, i.e., Dflow and T-funnel. This can be explained by the reduction on paste content. The factor Vw/Vp impacted fresh state properties

as expected, but with a positive effect. This as expected, since a high water content increase the flowability.  $V_w/V_c$  was by far the main factor determining the mechanical strength, both flexure and compression. In addition,  $V_s/V_m$  was also significant, but in this case a negative effect was observed. A significant quadratic term on  $V_s/V_m$  was also found Significant for Flexure strength.  $Sp/p$  exhibited the lowest influence on high performance self-compacting mortar properties. This can be explained by the short range of variation of  $Sp/p$  in the experimental plan, which was determined by the strong dispersion action of the superplasticizer used (Viscocrete 3008).

## 4 Conclusions

- Quadratic models were found to be adequate to describe the mortar properties – slump-flow diameter, V-funnel time, flexure and compressive strength – over the experimental region;
- $V_s/V_m$  was the main effect on the slump-flow diameter and V-funnel. An increase of  $V_s/V_m$  reduces the slump-flow diameter and t-funnel;
- $V_w/V_c$  was found to be the most influencing variable flexure and compressive strength. An increase of  $V_w/V_c$  reduces the flexure and compressive strength;
- $Sp/p$  exhibited the lowest influence on high performance self-compacting mortar properties, which might be explained by the limited range dosages employes in the current work;
- Numerical optimization allowed further improvement of the mortar properties in the fresh state and in terms of mechanical behaviour;
- DOE definitively is a power tool to better understand, optimize and design the mortar phase when very demanding performance requirements exists.
- The compressive strength model ( $R_c, 24h$ ), among the four obtained, was the one that best translated the results found.

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