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NUMERICAL PREDICTION OF THE COMPONENT-RATIO-DEPENDENT COMPRESSIVE STRENGTH OF BONE CEMENT

Abstract

Changes in the compression strength of the PMMA bone cement with a variable powder/liquid component mix ratio were investigated. The strength test data served to develop basic mathematical models and an artificial neural network was employed for strength predictions. The empirical and numerical results were compared to determine modelling errors and assess the effectiveness of the proposed methods and models. The advantages and disadvantages of mathematical modelling are discussed.

1. INTRODUCTION

The use of polymer biomaterials has become a common standard in a range of medical applications, including orthopaedic surgery and dentistry, where they are referred to as cements (Balin, 2004, 2016). In orthopaedics, they are predominantly found in joint arthroplasty and as a filler material in extensive bone defects.

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At present, in total joint replacement, prostheses are commonly fixtured with the PMMA bone cement (polymethyl methacrylate), which has been in use since 1960s (Charnley, 1960). Charnley, an early pioneer in modern arthroplasty, was the first to use the methyl methacrylate resin to bond endoprostheses (Balin, 2016; Matuszewski et al., 2014). Considering the applications of bone cements in medicine, the fundamental factors of their biofunctionality are as follows: carrying static and dynamic loads, dampening vibrations, abrasion resistance and biocompatibility (Balin, 2016; Wekwejt et al., 2019).

Given the aggressive operating environment, it is of great importance that bone cements are described in due detail with respect to their resistance to ageing processes and the resulting deterioration in strength (Lelovics & Liptakova, 2010, 2019; Matuszewski et al., 2014). Early loss of mechanical properties could cause endoprosthesis loosening and, thereby, necessitate revision surgery. These processes, i.e. the rate of ageing and depletion of mechanical parameters, can be contributed to several factors, including the mixing (Dunne & Orr, 2001; Lelovics & Liptakova, 2010; Liptáková, Lelovics & Necas, 2009), porosity (Dunne, Orr, Mushipe & Eveleigh, 2003; Pałubicka, Czubek & Wekwejt, 2019), contamination of cement with bone marrow, blood, Ringer's solution and other biofluids that by enabling micromovements, increase the risk of debonding at the bone-cement interface (Bialoblocka-Juszczyk, et al., 2008; Karpiński, Szabelski & Maksymiuk 2019a, 2019b; Tan, Koh, Ramruttun & Wang, 2016), or adding special-purpose admixtures into the cement structure (Wekwejt, Moritz, Świeczko-Żurek & Pałubicka 2018, Wekwejt et al., 2020).

Experimental investigations of ageing processes and changes in mechanical properties of biomaterials are cost-intensive let alone exceptionally time-consuming. The intrinsic limitations of empirical testing can be overcome using computer-aided methods, which exponentially reduce data collection and processing times and limit the required computational cost. As a result, they may help select or refine the optimal direction of further research. Numerical methods include predictive analytics, whose models enable the determination of relationships between corresponding parameters on the basis of experimental data (Younesi, Bahrololoom & Ahmadzadeh, 2010). Other analytical instruments of established computational prowess that have been put to use in this work, are the finite element method (FEM) (Falkowicz & Debski, 2019, 2020; Falkowicz, Debski & Wysmulski, 2020) and the boundary element method (BEM).

2. PREDICTIVE ANALYSIS

The performance of the selected analytical methods and tools was verified using statistical analysis and artificial neural network (ANN) modelling. The testing data were obtained from the results of the strength of bone cements in compression. The test specimens had been prepared with a variable amount of the liquid monomer

– one of the two components of bone cement – to evaluate how the changes in the PMMA cement composition by mass correlate with its strength performance (Karpinski, Szabelski & Maksymiuk, 2018, 2019a, 2019b). Two learning datasets were used for predictions and verification against the actual data (Fig. 1):

– the data from the range -30 % to +25 % served to predict the +35 % variant,
– the data from the range -20 % to +35 % served to predict the -35 % variant.

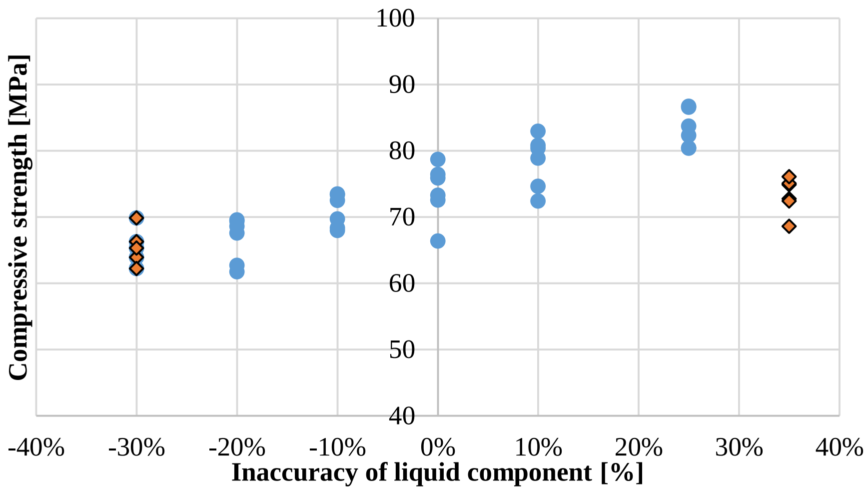

Fig. 1. Result from experimental research on compressive strength

Due to the physical nature of the investigated changes, it was resolved that polynomial models including linear would be most suitable to carry out the calculations, specifically, to determine the relationship accounting for the course of changes in the compressive strength in the specified range. The selected range is a slice of the entire hypothetical range from -100 % (no liquid component) to +∞ (only liquid component). From the logical analysis of the boundary conditions, it seems that, globally, the most appropriate is the quadratic polynomial model. In the model, which is a concave downward parabola, the maximum parameters are recorded in the middle of the range, and towards the edges, they decrease to the minimum (zero). However, in the tested range, it may emerge that one of the other models will perform with higher precision, both in terms of goodness of fit and prediction results.

2.1. Mathematical modelling of compressive strength

Statistical modelling was carried out using Microsoft Excel and Tibco Statistica software. It consisted in the analysis of relationships between variables, the determination of its linearity (regression) and approximation by means of the linear function and polynomials.

2.1.1. Excess of the liquid component (+35 %)

The generated mathematical models are as follows:

$$\sigma_{+35\_1} = 34.349x + 74.494$$
$$\sigma_{+35\_2} = 14.443x^2 + 34.963x + 74.026$$
$$\sigma_{+35\_3} = -108.11x^3 + 7.3284x^2 + 41.435x + 74.213$$
$$\sigma_{+35\_4} = 300.64x^4 - 71.069x^3 - 15.498x^2 + 39.628x + 74.376$$
$$\sigma_{+35\_5} = -8803.6x^5 - 1357.4x^4 + 634.85x^3 + 88.061x^2 + 31.816x + 73.878$$

where: σ – a modelled compressive strength of the cement sample, x – the liquid component excess (wt. %).

The model accuracy is assessed by the coefficient of determination R^2, and it displays a good correlation with the empirical results, which is confirmed by the following:

$$R^2(\sigma_{+35\_1}) = 0.7911$$
$$R^2(\sigma_{+35\_2}) = 0.7951$$
$$R^2(\sigma_{+35\_3}) = 0.7995$$
$$R^2(\sigma_{+35\_4}) = 0.7999$$
$$R^2(\sigma_{+35\_5}) = 0.8022$$

Having established that the models were of adequate predictive capacity, they performed the compressive strength simulations for the material with a +35% excess of the liquid part. The numerical data were subsequently verified using the mean results from the experimental tests:

$$\sigma_{+35\_1\_model} = 86.52\ MPa$$
$$\sigma_{+35\_2\_model} = 88.03\ MPa$$
$$\sigma_{+35\_3\_model} = 84.94\ MPa$$
$$\sigma_{+35\_4\_model} = 87.81\ MPa$$
$$\sigma_{+35\_5\_model} = 56.41\ MPa$$

while

$$\bar{\sigma}_{+35\_experimental} = 73.30\ MPa.$$

The root-mean-square error (RMSE) and its coefficient of variation (CV (RMSE)), accounting for the discrepancies between the predicted and observed values, were shown to attain notably higher values compared to the liquid component deficiency variant:

$$RMSE_{+35\_1} = 13.45, CV(RMSE_{+35\_1}) = 15.5\%$$
$$RMSE_{+35\_2} = 14.94, CV(RMSE_{+35\_2}) = 17.0\%$$
$$RMSE_{+35\_3} = 11.94, CV(RMSE_{+35\_3}) = 14.0\%$$
$$RMSE_{+35\_4} = 14.72, CV(RMSE_{+35\_4}) = 16.8\%$$
$$RMSE_{+35\_5} = 17.07, CV(RMSE_{+35\_5}) = 30.3\%$$

The models generated from the experimental data in the range from -30 % to approx. +25 % of the liquid component can be compared with the actual values for the predicted range of +35 % in Fig. 2.

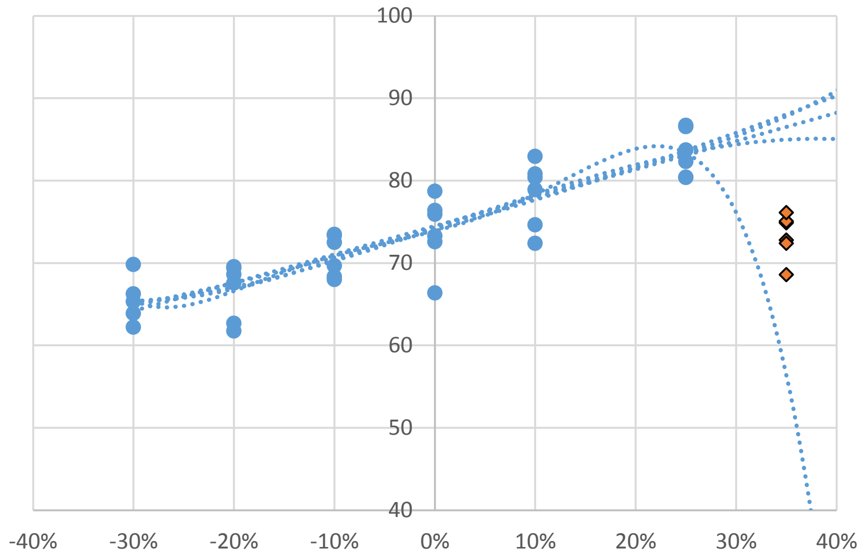

Fig. 2. Compressive strength of bone cement with a +35 % excess of the liquid component: comparison of mathematical models and experimental data

2.1.2. Deficiency of the liquid component (-30 %)

The methodology of computations is the same as in the former case. The following models were generated:

$$\sigma_{-30\_1} = 20.66x + 72.86$$
$$\sigma_{-30_2} = -57.226x^2 + 24.45x + 75.457$$
$$\sigma_{-30\_3} = -377.13x^3 - 30.207x^2 + 54.631x + 75.075$$
$$\sigma_{-30\_4} = -1015.5x^4 - 281.68x^3 + 77.675x^2 + 49.915x + 73.816$$
$$\sigma_{-30\_5} = -4304.9x^5 - 433.68x^4 + 286.35x^3 + 29.73x^2 + 35.211x + 74.165.$$

The goodness of fit of forecasted data with the actual results, assessed by the coefficient of determination, is not as high as in the previous case:

$$R^2(\sigma_{-30\_1}) = 0.4654$$
$$R^2(\sigma_{-30\_2}) = 0.5904$$
$$R^2(\sigma_{-30\_3}) = 0.7414$$
$$R^2(\sigma_{-30\_4}) = 0.7738$$
$$R^2(\sigma_{-30\_5}) = 0.7846$$

Compressive strength forecasting results:

$$\sigma_{-30\_1\_model} = 66.66\ MPa$$
$$\sigma_{-30\_2\_model} = 62.97\ MPa$$
$$\sigma_{-30\_3\_model} = 66.15\ MPa$$
$$\sigma_{-30\_4\_model} = 65.21\ MPa$$
$$\sigma_{-30\_5\_model} = 65.49\ MPa$$

while

$$\bar{\sigma}_{-30\_experimental} = 65.52\ MPa.$$

The RMSE and its coefficient of variation CV (RMSE), provide the description of the difference between predictions and actual strength of bone cement in compression:

$$RMSE_{-30\_1} = 2.81, CV(RMSE_{-30\_1}) = 4.2\%$$
$$RMSE_{-30\_2} = 3.61, CV(RMSE_{-30\_2}) = 5.7\%$$
$$RMSE_{-30\_3} = 2.64, CV(RMSE_{-30\_3}) = 4.0\%$$
$$RMSE_{-30\_4} = 2.58, CV(RMSE_{-30\_4}) = 4.0\%$$
$$RMSE_{-30\_5} = 2.57, CV(RMSE_{-30\_5}) = 3.9\%$$

Fig. 3 presents the results from the simulations, i.e. models generated from the empirical data limited to the range from -20 % to approx. +35 % of the liquid component content, along with the actual values for the predicted range of -30 %.

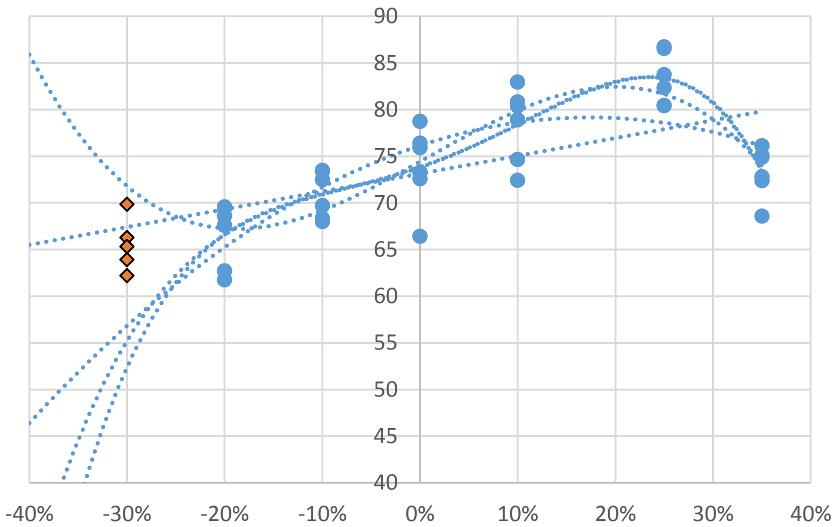

Fig. 3. Compressive strength of bone cement with a -35 % deficiency of the liquid component: comparison of mathematical models and experimental data

2.2. Artificial neural network forecasting

Deep learning neural networks (DLN) have been steadily becoming the standard among machine learning algorithms. Their advantages are demonstrated by their great capacity for capturing existing relationships between particular data – including performing calculations on extensive quantities of data, on numerous levels of abstraction. What distinguishes them from conventional NNs (Neural Networks) is that DLNs' operation is fully automated and does not require supervision or additional generalisation of features by human operators. DLNs are found in a range of applications, including speech recognition (Tu, Du & Lee, 2019; Zhang et al., 2019), image processing (Chen, Zhang, Liu & Kamruzzaman, 2019; de Haan, Rivenson, Wu & Ozcan, 2020; Hatt, Parmar, Qi & El Naga, 2019) or medical diagnosis (Hosseini, Hosseini & Ahi, 2020; Jiménez & Racoceanu, 2019; Lee et al., 2019).

In the works reported in this paper, the performance of DLN algorithms was compared with mathematical modelling. The procedure for analysing the effect of powder/liquid components mix ratio on the compressive strength of bone cements using DLN was the following:

- preliminary data preparation (alignment of the input data length),
- arranging data in the strings: -35 %, -25 %, -10 %, 0 %, +10 %, +20 % and +30 % of the cement mix component disproportion,
- inserting data into MATLAB (Deep Learning package with the Adam optimiser),

– testing in two variants: testing the predictive performance for a series of data from random samples and training the network on mean results (Fig. 4),
– the network architecture was: 50 hidden neurons and 150 iterations; to prevent overfitting, the dropout technique was employed and a gradient threshold was introduced.

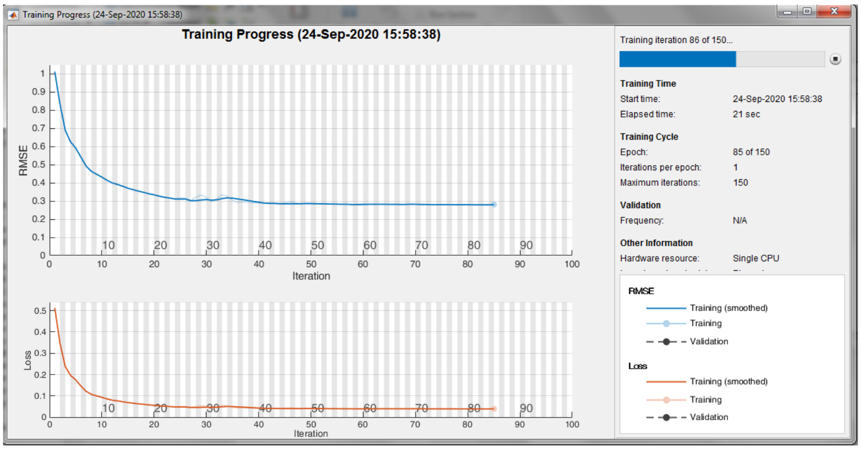

Fig. 4. Network training progress in MATLAB – RMSE reduction as a function of iteration

The compressive strength values predicted by the DLN network are presented below.

2.2.1. Excess of the liquid component (+35 %)

$$\sigma_{+35\_dln1} = 72.73\ MPa$$
$$\sigma_{+35\_dln2} = 69.83\ MPa$$
$$\sigma_{+35\_dln3} = 68.42\ MPa$$
$$\sigma_{+35\_dln4} = 69.56\ MPa$$
$$\sigma_{+35\_dln5} = 54.53\ MPa$$
$$\sigma_{+35\_dln6} = 64.00\ MPa$$

$$\bar{\sigma}_{+35\_dln} = 76.71\ MPa$$

$$SD\left(\sigma_{+35\_dln}\right) = 3.76\ MPa$$
$$CV\left(\sigma_{+35\_dln}\right) = 4.9\%$$

while

$$\bar{\sigma}_{+35\_experimental} = 73.30\ MPa.$$

2.2.2. Deficiency of the liquid component (-30 %)

$$\sigma_{-30\_dln2} = 77.67\ MPa$$
$$\sigma_{-30\_dln3} = 74.97\ MPa$$
$$\sigma_{-30\_dln4} = 78.49\ MPa$$
$$\sigma_{-30\_dln5} = 79.08\ MPa$$
$$\sigma_{-30\_dln6} = 80.10\ MPa$$

$$\bar{\sigma}_{-30\_dln} = 66.50\ MPa$$

$$SD\left(\sigma_{-30\_dln}\right) = 7.20\ MPa$$
$$CV\left(\sigma_{-30\_dln}\right) = 10.8\%$$

while

$$\bar{\sigma}_{-30_{experimental}} = 65.52\ MPa.$$

Subsequently, the results were analysed statistically and verified against the experimental data from the strength tests. Having proven the normality of data distribution, the analysis of variance confirmed their homogeneity and the Student's t-test, carried out at a confidence level $\alpha = 0.05$, indicated that the results from the neural network modelling were of good quality, that is regardless of the liquid component deficiency/excess variant. Therefore, given the lack of statistically significant differences, in the subsequent analyses mean network results were used.

3. DISCUSSION

Figures 5 and 6 display differences between mean values obtained from analytical investigations (DLN, mathematical modelling with polynomials) and values obtained from destructive physical analysis for both investigated variants of deviation from the correct powder/liquid component mix ratio.

From the comparison of Figures 5 and 6, a notable discrepancy emerges between the accuracy of predictions with respect to particular bone cement composition disproportions. Up to the level of +35 %, the excess of the liquid component is shown to have a positive effect on the material strength; after reaching the threshold limit, there is a steep drop in its resistance to loading in compression.

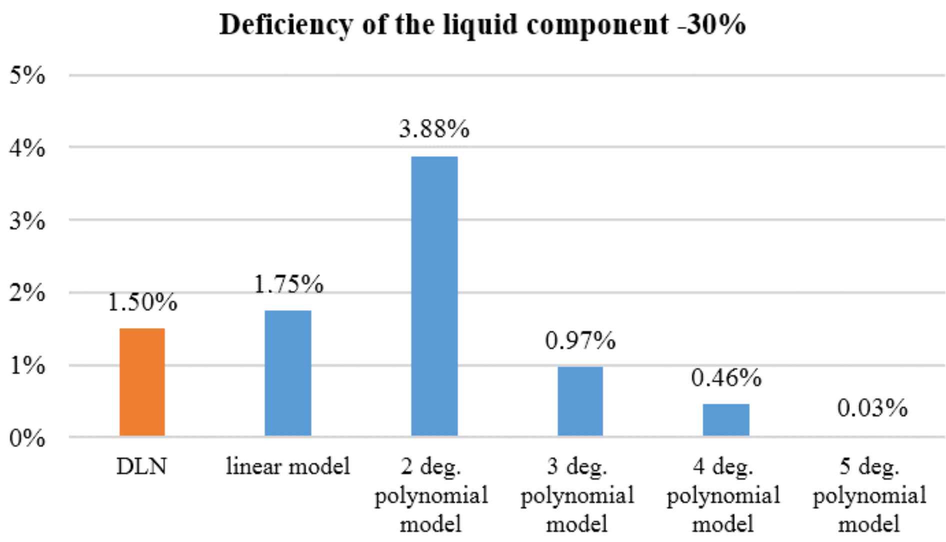

Fig. 5. Differences between modelled and actual compressive strength values for -30 %

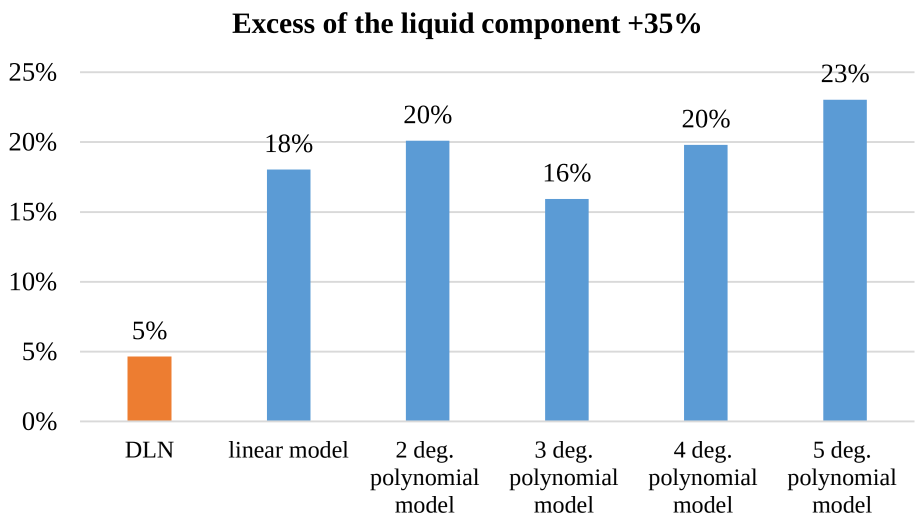

Fig. 6. Differences between modelled and actual compressive strength values for +35 %

Not entirely unexpectedly, the mathematical models have failed to forecast these tendencies, i.e. the differences between the predicted and the actual values were always in the excess of 15 %, regardless of the model (15–23 %) – Fig. 6. The result of mathematical computations can be thus merely treated as a useful forecast. However, these results may not be universally applicable to all situations, since the testing conditions were rather coincidental and perhaps non-replicable.

On the other hand, it is worth noting the exceptional predictive performance of the deep learning network, which displayed a slight, 5 %, error when correlated with the results from the strength tests. Thereby, the DLN outperformed the mathematical models and confirmed that the parameter change predictions from the latter are burdened with limitations, despite their good fit with the learning data. Furthermore, our findings appear to indicate that striving for the best fit is in itself insufficient to guarantee satisfactory predictive accuracy of the model. This is exemplified by Fig. 7, which compares the R^2 values (the coefficient of determination) of the subsequent models and the coefficient of variation of the root-mean-square deviation (CV (RMSD)), which describes the difference between the predicted and the observed values (with respect to the mean value).

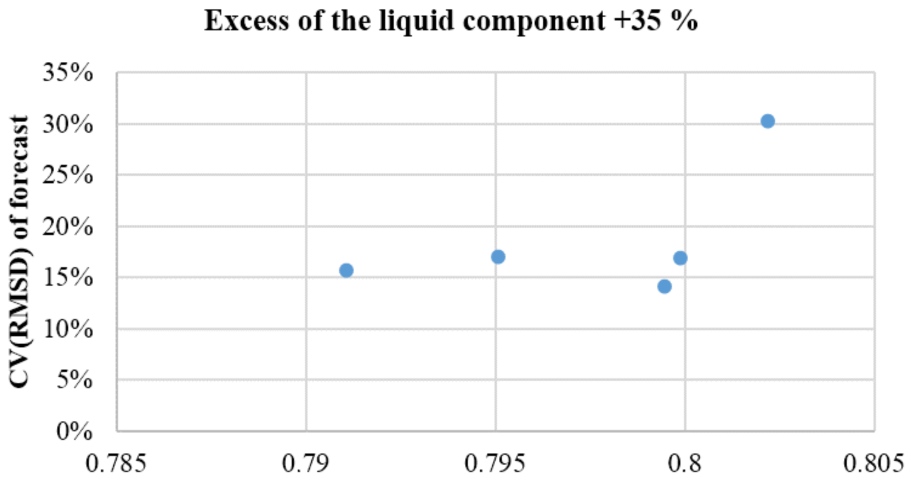

Fig. 7. CV(RMSD) vs R2 for +35 % forecasting

A notable increase in the quality of predictions was observed in the case when the -30 % variant of the liquid component deficiency was considered. The compressive strength values generated by the mathematical models did not exhibit a marked difference from the average values obtained experimentally (0.03–3.88% – within the margin of error), and the models can be, thus, considered as reliable predictors of the compressive strength of cement. As in the prior case, the DLN displayed good predictive capacity (a statistically insignificant difference of 1.5 % from the experimental value). Considering the deficiency of the liquid part, the strength parameter is shown to change in a more predictable way along with the decrease in the proportion of the liquid part. Similarly to the + 30 % variant, the model's goodness of fit was strongly correlated with the increase with each degree of polynomial approximating the results from the empirical tests. However, this correlation did not translate into more accurate results (Fig. 8).

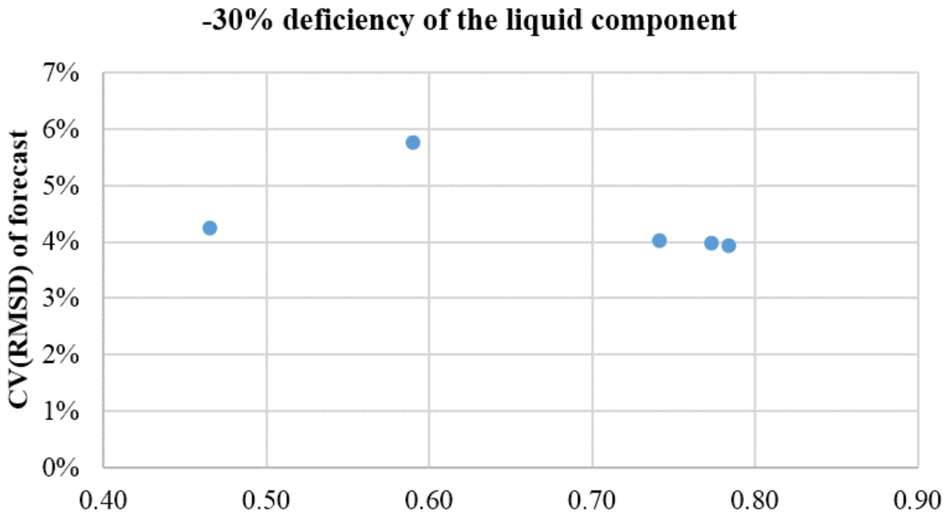

Fig. 8. CV(RMSD) vs R^2 for -30 % forecasting

5. CONCLUSIONS

The results of this investigation have shown that, in general terms, there is no consistent association between increasing the model/learning datasets' goodness of fit and an enhancement in the predictive accuracy of models. Furthermore, in spite of the improved values of coefficient of determination (with each degree of polynomial), the decrease in the root mean square error for the predicted values was negligible, or otherwise remained largely unchanged, except for rare cases of a slight increase. Therefore, based on our findings, there are no grounds to claim that even the best fit of the modelled and input data should guarantee a comparable level of predictive accuracy for values outside the range of the input data. Moreover, the learning data on the basis of which the models were generated, displayed a sharp change in the rising trend (considering the excess of the liquid component) above the +35 % level. This occurrence was found to severely hamper forecasting, as such a sudden drop is in principle impossible to predict when creating a mathematical model. This results in high uncertainty of the compressive strength values predicted with the use of the mathematical method. Interestingly, the artificial neural network exhibited a fairly high precision of compressive strength predictions despite the aforementioned problems. This may be indicative of an important capability of deep learning ANNs (DLN) to define relationships without the need to generalise their features. It is likely that the dropout technique (preventing overfitting) may have also played a significant role. From the point of view of their practical implementation, the choice of either of the described methods requires prior consideration and selection of the optimal modelling solution. What needs to be considered is that although the network may provide a better fit, the use of DLN may incur a high computational cost. That is why, in some applications, a simple linear model is a sufficient tool that will provide an acceptable level of predictive capacity.

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