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MATERIAL PARAMETERS OF CEMENT AND ALKALI ACTIVATED FLY ASH CONCRETE MIXTURES LABORATORY MEASUREMENTS AND NUMERICAL SIMULATION

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Abstract: *The paper reports on the determination of basic mechanical material parameters of several concrete and alkali activated concrete and fly ash mixtures intended for the construction of segmental lining used in TBM tunneling. The results of an extensive experimental program are discussed first. The principal attention is accorded to the experimental determination of specific fracture energy, which, when compared to numerical simulations, shows certain inconsistency with the measurements of other material data. This is supported by the derivation of the data from inverse analysis employing the elements of soft computing. Dynamic simulation of crack propagation experiments is suggested to reconcile the essential differences and to identify the most important impacts affecting the results of experimental measurements.*

Keywords: ***Alkali activated fly ash, Concrete, Fracture energy, Finite element simulation, Soft computing.***

1. Introduction

Massive increase of CO_2 emission in recent years has supported a considerable effort towards substitution of ordinary Portland cement by alkali-activated aluminosilicate materials such as fly ash in the production of concrete. Using fly ash as admixture in cements is now common in many applications. Full substitution for large scale structural units, however, is still at its infancy and to foster its progress beyond laboratory samples will require fundamental understanding of what is occurring already on the level of paste during alkali-activation process. Starting with recent accomplishments by Smilauer et al. (2011) we expect considerable activity in this field in the coming decade.

This topic, however, goes beyond the present scope. Instead we focus our attention on the macroscopic evaluation of the response of various mixtures of concrete and alkali-activated materials with emphases on the influence of fly ash replacing either a certain portion or an entire amount of cement. We report on both experimental and numerical part of this research effort as these should be considered on the same footing to mutually corroborate the obtained results.

Motivated by possible applications of these mixtures in the production of the segments of lining often used in hostile environment we set up an extensive experimental program that includes on the one hand small scale laboratory measurements of basic material parameters, material degradation due to activity of acid solutions, and on the other hand full scale measurements of resistance of lining segments to fire.

The present contribution is limited to the first part of this program aiming at quantification of individual mixtures with regard to their mechanical material data in the light of the required strength corre-

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sponding to concrete C50/60. The results of numerical simulations of selected tests are also present to warn engineers against blindly accepting the provided laboratory data which might not be suitable for intended numerical analysis on a structural level.

The remainder of this paper is organized as follows. Section 2. provides the list of examined mixtures. The results of experimental investigation are summarized in Section 3. Numerical part embracing also the identification of material parameters based on fracture energy measurements is described in Section 4. Brief summary is finally provided in Section 5.

2. Concrete and alkali activated mixtures

We begin by providing the list of examined concrete and alkali activated mixtures. Eight mixtures in overall were proposed. Two mixtures in particular assumed total replacement of concrete by fly ash activated by strong alkaline liquids such as a mixture of NaOH pellets dissolved in tap water and sodium silicate in the form of water glass. Low-calcium fly ash coming from the Mělník (FAM) and Opatovice (FAO) thermal electric power plants, the Czech Republic was used. Half the mixtures were further modified by adding 0.5% of volume of synthetic fibers Forta-Ferro. This amounted to 4.5 kg of fibers per 1 m^3 of the mixture.

The following notation is introduced to distinguish individual mixtures: C - Cement based concrete (reference mixture), POP - Alkali-activate fly ash, Fi - mixture containing fibers, FAC-1(2) - mixtures with partial replacement of concrete by fly-ash. All the mixtures considered the same grading curve. Specific fractions of stone grains are listed in Table 1. Individual mixtures are stored in Table 2.

Tab. 1: Fraction of grains

Fraction	Amount per 1 m^3 of mixture in [kg]
0/4	705
3/8	130
8/16	865

Tab. 2: List of selected mixtures

Material	Amount per 1 m^3 of mixture in [kg]			
Mixture →	C	FAC-1	FAC-2	POP
CEM I 52,5 R	460	322	322	-
limestone powder	40	40	40	-
Water	150	150	187	51
Fly ash		138 (FAM)	276 (FAM)	400 (FAO)
NAOH	-	-	-	29,4
Water glass 34%	-	-	-	127,5
Slaked lime	-	-	-	12
Glenium ACE	4.2	4.2	4.2	12

It will be seen in the next section that all cement based mixtures exceeded the required compressive strength of 50 MPa. Inability of alkali-activated mixtures (POP, FiPOP) to reach this value can be attributed to the insufficient curing temperature of about $40-45°$C which was chosen to meet the massive production feasibility.

3. Experimental program

Standard laboratory measurements were carried out at the Klokner Institute in Prague to obtain elastic moduli, cubic compressive strength and strength in transverse tension. While cubic specimens having edge length of 150 mm were used to measure strength properties ($f_{c,cube}$, f_t), $300\times150\times150$ mm prisms were manufactured to acquire the values of Young's moduli. These specimens were further utilized to provide the uniaxial compressive strength $f_{c,prism}$. All measurements were performed 28 days since the time of their production. The results appear in Table 3.

Tab. 3: Material properties

Notation	Elastic modulus	Compressive strength	Transverse tension strength	Fracture energy
	E [GPa]	$f_{c,cube}/f_{c,prism}$ [MPa]	f_t [MPa]	G_f [N/m]
C	38.5	84.7 / 72	4.4	207.4 220.3, 190.3
FiC	39.5	78.0 / 65	3.7	-
FAC-1	40.1	66.3 / 59	3.1	190.9
FiFAC-1	39.7	61.3 / 63	3.1	-
FAC-2	-	54.0* (71.0**)	-	-
FiFAC-2	-	48.2* (69.9**)	-	-
POP	18.9	36.2 / 28	2.9	112.3
FiPOP	20	39.5 / 30	2.9	-

To address the expected pozzolanic reaction the samples corresponding to mixtures FAC-2 and FiFAC-2 with increased amount of fly ash were tested after 60 ($*$) and 180 ($**$) days of curing. The measured values of cubic strength confirm the ongoing pozzolanic reaction even without alkaline activators. Unfortunately, the applicability of structural elements made from these mixtures might be limited by low strength at early time of curing.

3.1. Specific fracture energy

A particular attention was dedicated to the determination of fracture energy from a three-point bending test displayed in Fig. 1(a). Three notched specimens for each mixture having dimensions $150 \times 150 \times 700$ mm with a notch depth of 25 mm were tested in a displacement-controlled loading regime at the rate of 0.05 mm/min up to 0.2 mm of crack mouth opening displacement (CMOD) and at the rate of 0.2 mm/min until failure. Averages calculated for individual mixtures are available in the last column of Table 3. Although specimens containing fibers were also tested, the corresponding values are not provided owing to the uncertainty in the calculation of this value from associated loading diagrams. Some representatives are plotted in Fig. 1(c) showing relatively large residual strength up to 30% of the peak value.

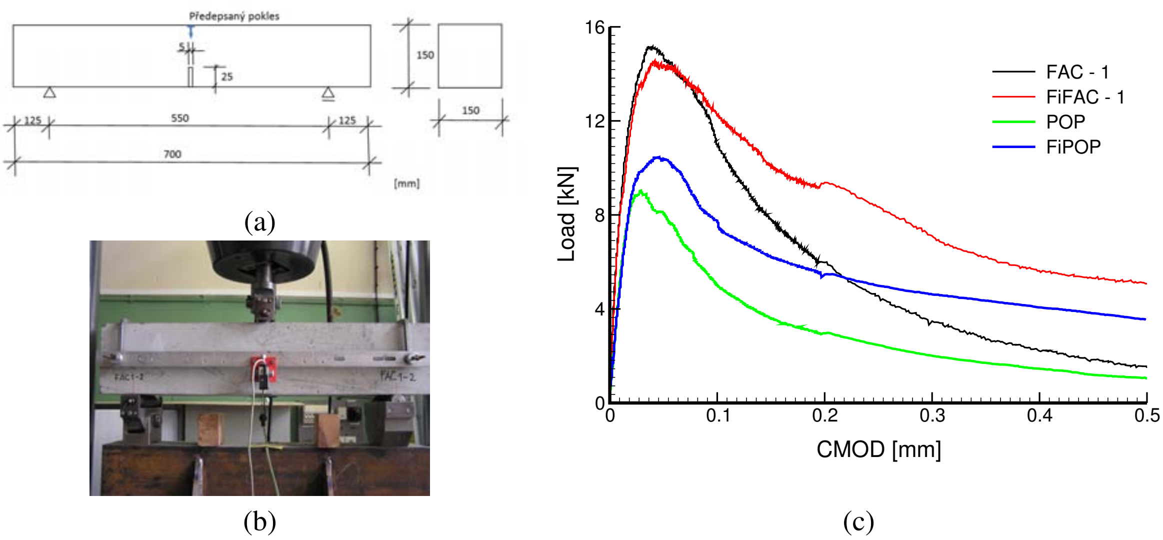


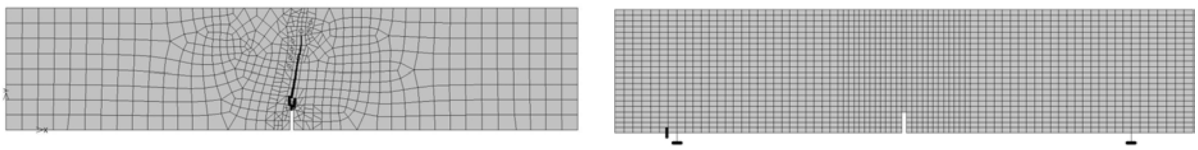
Fig. 1: Three-point bending test: (a) Computational scheme, (b) Experimental set-up, (c) Selected loading diagrams

4. Numerical simulation

This section offers the possibility of estimating the material parameters from fracture-mechanics tests by matching the experimentally measured and numerically derived loading curves. At the same, it raises a number of questions regarding the reliability of the results provided by either of the two methods if these are not mutually corroborated. The macroscopic loading curves of two selected concrete specimens denoted as C1 and C2 plotted in Fig. 3 as black solid lines were selected as our point of departure.

4.1. Static simulation of fracture energy test

To begin with, we adopted a simple trial and error method. The associated results stored in Table 4 are labeled as IDTE Mesh-TE where Mesh-TE denotes the finite element mesh seen in Fig. 2(a).



(a) (b)

Fig. 2: Finite element meshes adopted in numerical simulations: (a) Mesh-TE, (b) Mesh-NN

The ATENA finite element code (Červenka et al. (2007)) was used to simulate the three-point bending test numerically. A 3D Non Linear Cementitious 2 material model was selected to govern the gradual evolution of localized damage. The model is formulated in the total format assuming small strains and initial isotropy of a material. The tensile behavior is governed by the Rankine-type criterion with exponential softening while in compression, the Menétrey-Willam yield surface with hardening and softening phases is used. The fracture model employs the orthotropic smeared crack formulation and the fixed crack model with the mesh adjusted softening modulus. This model is defined on the basis of characteristic element dimensions in tension and compression to ensure the objectivity in the strain-softening regime. The required material parameters are presented in Table 4

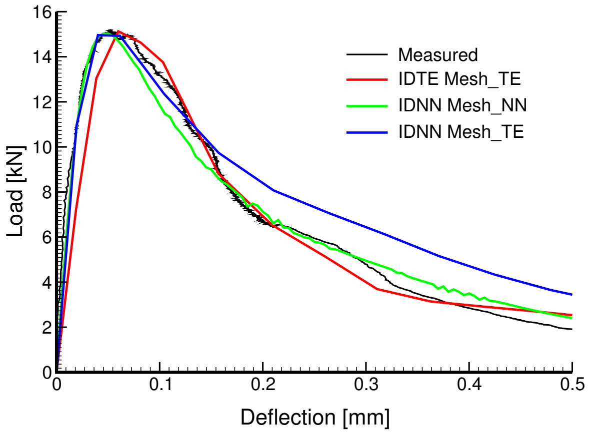
Tab. 4: Material data of 3D Non Linear Cementitious 2 model for two specimens C1/C2

Parameter	IDTE Mesh-TE	IDNN Mesh-NN	IDNN Mesh-TE
Elastic modulus [GPa]	48 / 55	82* / 96*	82 / 96
Poisson's number [-]	0.2	0.2	0.2
Tensile strength [MPa]	3.8 / 4.5	2.7* / 2.9*	2.7 / 2.9
Compressive strength [MPa]	72	72	72
Specific fracture energy [N/m]	70 / 60	228* / 206*	228 / 206
Specific weight [kN/m^3]	24.7	24.7	24.7

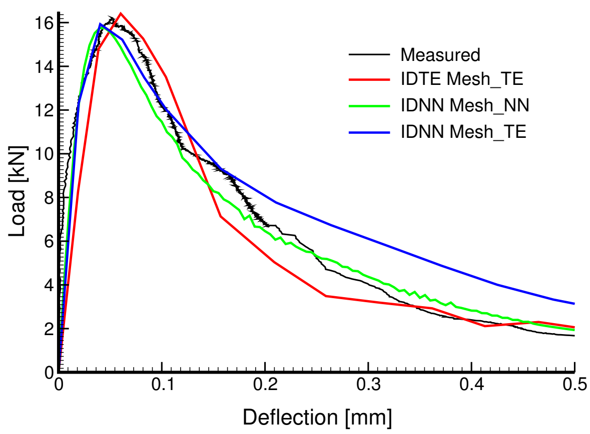
The material parameters employed in this case study are introduced in the first column of Table 4 (IDTE Mesh-TE). The objective was to use the experimentally obtained data if possible while attempting to match the available loading curves. While the Young's moduli and tensile strengths received only minor adjustment if compared with the measured values in Table 3, the specific fracture energy required a significant reduction to match measured and simulated loading curves reasonably close; compare the black and red solid lines in Fig. 3. Compare also model fracture energies in the 1st column of Table 4 and the corresponding ones available in the 2nd row of Table 3. These results are the first indication as to the inadequacy of the measured fracture energy to be used as a geometry independent material parameter in full scale structural simulations.

4.2. Numerical derivation of material data from inverse analysis

Quite severe deviations between measured and numerically estimated specific fracture energies provided by a simple direct approach promoted the application of a more rigorous type of inverse analysis adopting



(a)



(b)

Fig. 3: Measured and numerically derived loading curves for two concrete specimens: (a) C1, (b) C2

the elements of soft computing (Novák and Lehký (2006); Lehký and Novák (2009)). Herein, we report on the approach combining artificial neural network (ANN) and finite element method.

Again the ATENA code was used to perform numerical simulations. The corresponding finite element mesh appears in Fig. 2(b). Based on sensitivity analysis (Novák et al. (1993)) we considered Young's modulus E, tensile strength f_t and specific fracture energy G_f be subject to identification. These are labeled with (*) in Table 4. Other material data were assumed fixed either provided by experiment such as the compressive strength $f_{c,prism}$ or assigned default values offered by the program for the selected material model.

As for the searching strategy, the implemented artificial neural network is of a feed-forward multilayer type. The network consisted of 3 inputs, one hidden layer having 5 neurons with non-linear transfer function (hyperbolic tangent) and output layer having 3 neurons with a linear transfer function. Each of the output neurons corresponds to one of the identified parameter. The size of training set was set to 50 samples generated using the Latin Hypercube Sampling method (McKay et al. (1979)). To train ANN Levenberg-Marquardt optimization method (Singh et al. (2007)) and genetic algorithms (Haupt and Haupt (2004)) were used. Once ANN was trained the experimental response was used to obtain identified parameters. With this set of parameters numerical analysis was carried out and resulting response was compared with the experimental one. The resulting loading curves corresponding to identified parameters in Table 4 are plotted as solid green lines (IDNN Mesh-NN) in Fig. 3.

Note that while the identified values of G_f are in a very good agreement with those provided by experiment, recall the 2nd row in Table 2, the identified values of Young's moduli are unrealistically high especially when compared to the measured ones. Further indication suggesting that the measured values of fracture energy can hardly be accepted as material parameters for structural analysis is a strong dependence of the results on finite element mesh evident from plots in Fig. 3, blue solid lines labeled as IDNN Mesh-TE. These were found after running the numerical analysis with identified data but adopting the unstructured coarse mesh in Fig. 2(a). It is reasonable to expect that for large scale structural analysis the adopted finite element mesh would be even coarser.

4.3. Dynamic simulation of fracture energy test

Learning from experience (Keršner et al. (2011)) a number of issues might be examined to provide solid explanation for inconsistency between experimental results and numerical simulations. The principal impact factor affecting the experimental results can be attributed to the relatively fast rate of loading which should be reflected in numerical simulations by accounting for inertia properties of the components of loading test setup. Dynamic simulation of the crack propagation test discussed already by Frantik (2008) can provide explanation to a high initial stiffness, recall the results of identification analysis, by incorporating the viscous damping of the specimen. This causes a slower stress distribution inside of the specimen and consequently leads to higher forces during fast loading. Other issues worth of future investigation include significant oscillations of time series of vertical displacements, unsymmetrical bending, etc.

5. Conclusions

The present contribution summarizes the experimental part of the project concerned with the modeling of TBM based tunneling in densely populated areas. Emphases were given to the experimental investigation of several cement and alkali activated fly ash based concrete mixtures. With principal attention paid to the specific fracture energy we attempted to confirm the experimental measurements by an independent numerical simulation of a three-point bending test employing the ATENA finite element code. Both simple trial and error method as well as more rigorous ANN based identification method were exercised. Both approaches revealed unreliability in the direct use of experimentally measured values of fracture energy as a material parameter. Most probably, this could be attributed to the applied rate of loading, which should be at least $10\times$ smaller to comply with the assumption of static analysis generally neglecting the viscous effects. This issues will be the subject of further research. Attention also deserves a considerable dependence of the results of simulations on the finite element mesh promoting similar mesh coarseness used in lab experiments and structural simulations at least in areas prone to damage evolution.

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