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Multiscale model for the prediction of equation of state for cement paste and mortar

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ABSTRACT

The behavior of cementitious materials under severe loading is of major importance for the security protection of concrete structures. One of the key mechanical properties of materials subjected to extremely high loading is the relationship between hydrostatic pressure and volumetric strain, which is often referred as the equation of state. In porous materials such as cement paste and mortar, this relationship is substantially inelastic due to the closure and collapse of capillary pores. At extremely high pressures, after all pores are closed, the equation of state approaches the elastic properties of the matrix. This paper presents an updated theoretical model of the equation of state of cement paste and mortar using a multi-scale approach. At the micro-scale level, an elastic-plastic spherical domain is considered with a single concetrical spherical cavity. The updated model includes a strain-hardening flow rule to describing the plastic closure of pores. At the macro-scale level, it is assumed that every differential spherical domain has random radial parameters following a realistic distribution function of pore sizes. The equations of state of the fine aggregates are assumed linear elastic and Hirsch phase mix rule is applied to obtain the equation of state of the composite material. All phases are assumed to be subjected to hydrostatic pressure. An extensive experimental study was conducted to calibrate and validate the proposed model. The comparison shows good agreement between the present model and the measured data.

1. Introduction

The behavior of cementitious materials under severe loading is of major importance for the security protection of concrete structures (Dancygier et al., 2007; Forrestal et al., 2003; Rosenberg and Dekel, 2016). Loads of extreme intensity caused, for instance, by impact and nearby explosions, produce in concrete structures extremely high tri-axial stresses (Grisaro and Dancygier, 2017; Mu et al., 2012). Accordingly, equation of state (EOS), which is pressure-volumetric strain relationship, plays a key role in the prediction of concrete behavior under such extreme loading and design of protective structures (Yankelevsky, 2017).

The behavior of concrete under high to extremely high pressures has not been investigated widely due to the complexity of the phenomena involved and to the need of special equipment for appropriate experimental studies. For this reason, the mechanisms of concrete deformations and damage under extremely high multi-axial stresses are far from being clearly understood.

Recent experimental research data, based on Split-Hopkinson pressure bar (SHPB) tests (Bragov et al., 2012; Gebbeken et al., 2006) as well as on extreme high-capacity triaxial pressure tests (Burlion et al., 2001; Cui et al., 2017; Poinard et al., 2012, 2010; Vu et al., 2009a, b, c), indicate a principal change in the behavior of concrete under high pressures. In contrast to its brittle behavior and localized damage under uniaxial stresses, concrete exhibits very high ductile resistance and diffused damage under extremely high hydrostatic stresses (Forquin et al., 2007; Gabet et al., 2008). It was demonstrated that high stresses are associated with considerable compaction, resulting from the closure of pores in the concrete (Burlion et al., 2001; Dupray et al., 2009). The development of an EOS appropriate for cementitious materials that considers confinement of pores due to the action of extremely high hydrostatic pressures is the subject of current research. The major approaches to modeling the concrete bulk behavior under extreme loading are presented below.

The simplest approach is based on the assessment of an EOS containing several parameters that are obtained by fitting to experimental test results. The best known examples of such EOS are the Shock-Hugoniot (Chen et al., 2001; Gebbeken et al., 2006; Grady, 1996), Tait –Murnaghan, and Tillotson EOS (Bažant et al., 2000) for dry materials and the P∼α EOS (Feldgun et al., 2014;

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Herrmann, 1969; Lyakhov and Okhitin, 1977; Riedel et al., 2009) for multi-phase materials. This approach considers only the macro-scale level behavior and need to be individually calibrated by experiment for each material.

Another approach is to take into consideration the microstructure of the cementitious materials by a multi-scale model. This can be done by for instance continuum damage theory coupled with a plasticity model (Cui et al., 2018; Dupray et al., 2009; Vu et al., 2010), or exploiting a discrete element modeling (DEM) (Tran et al., 2011). The former approach combines damage mechanics and a plasticity model of concrete in order to construct its EOS. In this model, the damage description is based on the continuum damage theory (Mazars, 1986; Mazars and Pijaudier-Cabot, 1989). The KST (Krieg-Swenson-Taylor) model (Krieg, 1972; Swenson and Taylor, 1983) was used for prediction of the concrete plastic deformations. Although this model considers the damage plasticity of cement mortar in combination with a linear elastic behavior of the aggregate, it does not include the debonding of aggregate from the cement paste matrix. Furthermore, an effective elastic modulus value of 35 GPa was used for the aggregates instead of a realistic value of 70 GPa in order to fit calculation results (Dupray et al., 2009; Malecot et al., 2010).

The DEM is a conceptually different approach to the numerical simulation of concrete. Tran et al suggested to utilize a three-dimensional DEM to predict the triaxial behavior of concrete under high-confining pressures (Tran et al., 2011). The interaction rules between the discrete elements should be defined by local constitutive parameters that need to be fitted by experimental data in order to reproduce a real concrete behavior. Among these interaction parameters is a local elastic-hardening damage constitutive law.

The first approach has relative simplicity and can be easily used for the implementation of traditional calculation methods of continuum mechanics. The second method allows taking into account some of the microstructural properties of the material. Nevertheless, both approaches have a considerable practical shortcoming. In both cases, calibration is required for each concrete composition by means of experimental data that are not always available. In most cases, the modeling parameters do not have physical meaning or relationship with the composition or mechanical properties of real concrete properties. For this reason, these parameters cannot be calculated based on the mix proportions of concrete or simple standard testing. Commonly, these simple models do not take into consideration major microstructural changes that have been established by experimental observations, for example, confinement of pores, debonding and cracking at the interface of aggregate and cement paste.

It should be noted that the extreme loading in the aforementioned problems is dynamic. Therefore, in the constitutive equations, it is necessary to consider the effect of strain rate. Nevertheless, this factor is theoretically more important in the deviatoric behavior and, in many cases, can be disregarded in the formulation of equation of state (Bažant et al., 2000; Bourne et al., 2008; Herrmann, 1969; Lindgren et al., 1999; Riedel et al., 2009).

A new multi-scale microstructural model for the quantification of the equation of state has been recently proposed (Karinski et al., 2015; Karinski et al., 2017c). This model considers the confinement of pores caused by exterior hydrostatic pressure. At the micro-structural scale level, it utilizes a simplified representation of a capillary pore in a cement paste matrix as a spherical void. The macro-scale level is obtained by averaging, taking into consideration stochastic distribution of both pore sizes and spatial arrangement of pores. Hirsch phase mix rule is applied to obtain the equation of state of the composite material, assuming fine aggregates been linearly elastic. This model demonstrated good results, but with some deviations from the measured experimental data, probably due to the elastic-ideally plastic assumption related to the cement paste matrix. This simplified assumed behavior of the matrix - without hardening - was aimed in order to obtain an analytical solution at the microscale level. This paper presents an updated model where the analytical solution of the micro domain considers an elastic linearly hardening plastic matrix behavior. The solution is obtained by using the Fredholm integral equation of the second kind utilizing Neumann series. The updated model is compared with experimental data and good agreement between the new model and the measured data is demonstrated. Note that the discussed model considers only cement paste and mortars. If concrete is to be considered, the coarse aggregates should also be described by an appropriate non-linear bulk behavior (Piotrowska et al., 2014).

2. The model outline

In the current model development, we utilized a multi-scale approach for the prediction of the loading branch of the equation of state for an unsaturated cement paste. The microscale level deals with the cement paste matrix spherical domain with a centered single void representing a capillary pore. The novelty of the proposed model is in taking into account the plastic hardening of the cement matrix as opposed to the ideal plastic behavior assumed in the previous model (Karinski et al., 2017c) aiming at better describing the gradual stiffness changes during loading. The macroscale level of the cement paste is acquired by averaging of the elasto-plastic solutions of the micro-domains considering spatial stochastic distributions of pores (Lu and Torquato, 1992) based on simplified pore-size distribution (Koenders and van Breugel, 1997a). The equation of state of mortar is obtained using Hirsch's phase mix rule (Hirsch, 1962).

3. Micro-scale level

Consider an elasto-plastic spherical domain having a concentric single spherical void with outer and inner radii Ro and Ri, respectively (see Fig. 1a). The solid matrix is considered an elasto-plastic isotropic material with linear plastic hardening. The domain is loaded by a hydrostatic pressure P at its outer boundary, while the inner boundary is pressure free. The positive compressive pressure rule was thereafter generally adopted. Here we assume a homogeneous stress field in the macro-domain, i.e the external pressure applied to macro-domain acts on the micro-domain as shown in Fig. 1.

Generally, four stages of the micro-domain deformation are recognized:

(i) Small elastic deformation at the early stage of loading (Fig. 1a);
(ii) Small elasto-plastic deformation with linear hardening during which the plastic zone propagates towards the outer boundary (Fig. 1b);
(iii) Plastic deformation encompasses the entire domain during which increasing large strains lead to complete void closure (Fig. 1c);
(iv) After the void closure, the micro-domain is in a hydrostatic state of stress and its bulk behavior is linear elastic with the properties of solid matrix (Fig. 1d).

The solution for small elastic deformations of a hollow sphere under external pressure is well known in the literature, e.g. see (Timoshenko and Goodier, 1951):

$$\sigma_r = -P\,\frac{R_o^3}{R_o^3 - R_i^3}\left(1 - \frac{R_i^3}{r^3}\right)$$

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