Simulation of Macroscopic Behavior of a Self-Compacting Mixture based on DEM

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ABSTRACT:
Since the early 20th century, the necessity of modeling and monitoring fresh concrete behavior has been recognized by the industry with the objective to ensure adequate mechanical properties and a proper durability of concrete structures.

Due to the rapid development of computer technology, the applications of computational simulation tools in the field of concrete technology has significantly increased and help us to understand the mechanisms of rheological systems. The development of proper rheological models and suitable numerical methods are considered as basic needs for a thorough understanding of the flow properties. The main challenge is finding a quantitative correlation between the model parameters and the properties and proportions of the mix ingredients.

This paper presents a numerical approach for macroscopic behavior of a fresh self-compacting mixture using Discrete Element Method (DEM). The employed research is based on a conceptual idea where the grain-paste interaction is explicitly modelled as an interactive two-phase system. Each mixture is considered to be an assembly of “grain-paste” systems, which can be characterized according to the mix composition based on the “excess paste theory”. The macroscopic behavior is evaluated based on the slump flow test results. Simulations and experimental laboratory test results show good agreement.

Keywords: Discrete element method (DEM), excess paste theory, flow analysis, fresh self-compacting mixture, slump flow test, two-phase element, two-phase model

INTRODUCTION

Due to the rapid development of computer technology in recent decades, the use of computational simulation tools in the field of concrete technology have been increased to a large extent[1]. For these simulations, mechanisms and parameters which influence the flow behavior should be expressed by a set of mathematical equations. There are two main approaches for flow analysis of a granular-paste material, i.e. a continuous and a discontinuous approach [2].

According to the continuous approach, concrete is considered as a homogeneous continuous fluid and its behavior is studied in the framework of continuum mechanics. The viscoplastic finite element method (VFEM) and the viscoplastic divided space element method (VDEM) are two well-known methods of that characterize this category [3, 4]. The assumptions associated with continuous media modeling turned out to be accurate enough to simulate materials like Newtonian liquids or ideal solids, but it is not an appropriate method for simulating a heterogeneous material like a concrete mixture, which consists of a wide range of ingredients that exhibit a unique ingredient-dependent behavior [5].

According to the discontinuous approach, concrete is considered as a heterogeneous multi-phase material (in the most cases, an aggregate/paste or coarse aggregate/ mortar system). An appropriate numerical method for the flow analysis of heterogeneous materials is based on a discontinuous approach, called the discrete element method (DEM) [6, 7]. This method is considered to be the most suitable method for investigating the macroscopic behavior from a microscopic perspective (local interactions between mix components)[1, 4].

In this study, concrete is considered as a two-phase system, i.e. aggregate and paste, and simulations are conducted with the particle flow code 2D of Itasca [8] which works based on discrete element Method (DEM).

MIX CHARACTERIZATION

In this study a fresh self-compacting mixture is considered as a discontinuous system and it is characterized by a two-phase model. These phases are aggregates and paste (see Figure 1). The granular phase is characterized by its packing density (ς). The packing density is expressed as follows:

$$\varsigma = \frac{\rho_b}{\rho_s} \qquad 1$$

where ρ_b and ρ_s are the bulk density and the specific density of the aggregates, respectively. The bulk density of the granular phase can be determined according to ASTM C 29 [9], while ASTM C 127 [10] and ASTM C128 [11] can be used for calculation of the specific density of the aggregates.

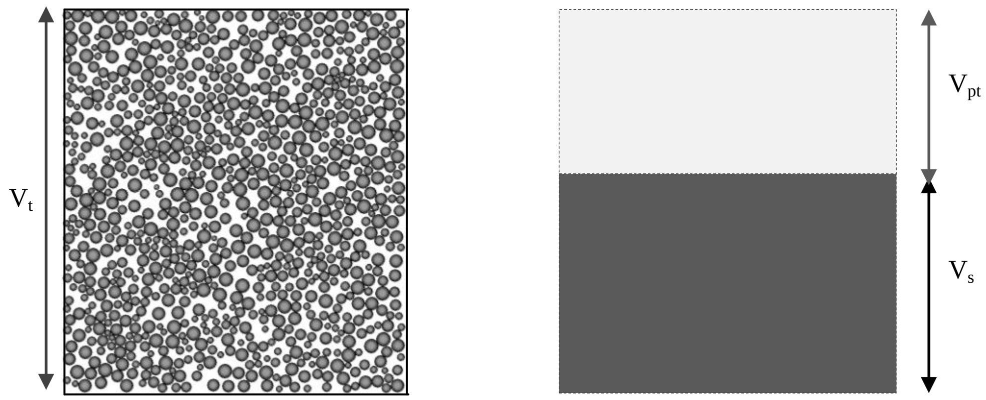
The paste phase is divided into two parts: 1) void paste and 2) excess paste. The void paste is the part of the paste filling the void space between the aggregates in fully optimized packing state (see Figure 1(b)). The excess paste is the part of the paste used to form a layer with constant thickness around each individual aggregate particle (δ_{pex}) (Figure 1(c)).

The paste fraction that corresponds to the void volume (V_{pv}) can be calculated with Equation 2:

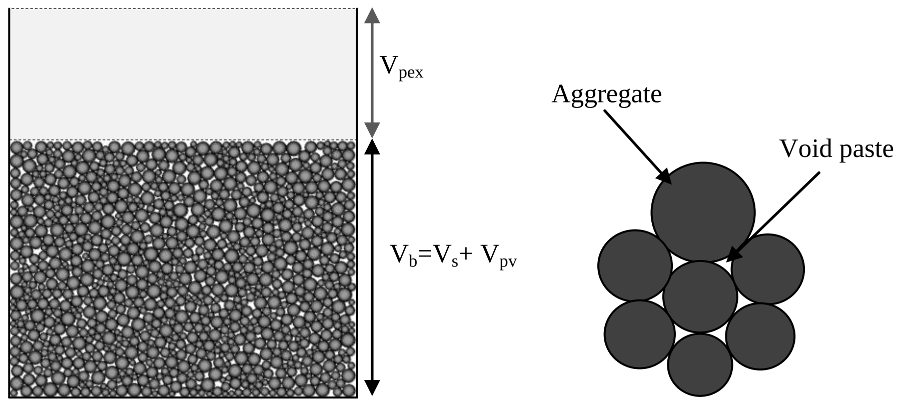
$$V_{pv} = (\frac{1}{\varsigma} - 1).V_s \qquad 2$$

where ς and V_s represent the packing density and the solid volume (aggregate volume) in a unit volume of granular skeleton. The volume of the excess paste (V_{pex}) is calculated by subtracting V_{pv}, the volume of the void paste, from V_{pt}, the total volume of the paste, as shown in Equation 3:

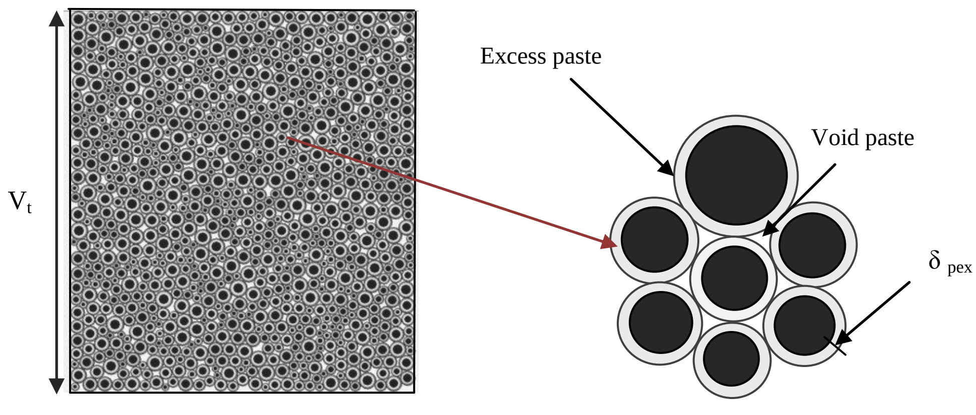
$$V_{pex} = V_{pt} - V_{pv} \qquad 3$$



(a) Loosely packed aggregates



(b) Fully optimized packing of aggregates



(c) Packing of aggregates corresponding to two-phase model

Figure 1 — Two-phase model for a fresh self-compacting mixture. In this figure V_t, V_b, V_{pt}, V_{pv}, V_{pex}, V_s and δ_{pex} stand for volume of the sample, bulk volume of the aggregates in fully optimized packing state, total paste volume, void paste volume, excess paste volume, volume of the aggregates and thickness of the excess paste layer, respectively.

In the calculation procedure of the thickness of the excess paste, it is presumed that the shape of the grain particles is spherical and the thickness of the excess paste around the particles is the same for all particle sizes. The latter presupposes a homogeneous dispersion of the grain particles in the mixture leading to a constant surface to surface distance between the particles. Under these considerations, the specific volume of granular skeleton (V_s) and the excess paste thickness (δ_{pex}) can be calculated by Equation 4 and Equation 5, where R_i and N_i represent the radius of particles of class i and the number of particles per class i, respectively.

$$V_s = 4/3.\pi. \sum N_i R_i^3 \quad (4)$$

$$V_{pex} = 4/3.\pi. \sum N_i ((R_i + \delta_{pex})^3 - R_i^3) \quad (5)$$

To characterize a fresh concrete mixture by this model, the rheological behavior of the mixture can be described qualitatively by the excess paste theory introduced by Kennedy[12]. According to this theory, the rheological behavior (degree of workability) is controlled by the solid-paste interactions through the excess paste layers, which can be characterized by the consistency of the cement paste and thickness of the excess paste layer. By increasing the consistency of the cement paste phase and the excess paste volume a higher degree of workability would be expected for a given concrete mixture.

FLOW ANALYSIS

The Discrete Element Method (DEM) is considered a computational technique that is used in this study. Based on this method, the material is built up of a finite number of individual elements (Figure 2). The macroscopic behavior of such a system is described in terms of the movement of elements and their inter-element interactions [13]. In DEM, the numerical representation of the deformation is performed through a time-stepping algorithm. During each cycle, first the set of contacts between elements is updated from the known positions of the elements. Then the interaction law is applied to each contact to update the resulting force and moment acting on each element based on the relative motion between the two entities. Finally the law of motion is applied to each element to update its velocity and position based on the resulting force and moment, arising from the interaction and body forces, acting on the elements [8].

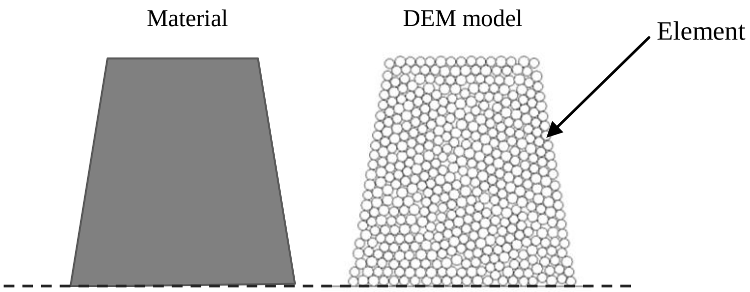


Figure 2 — DEM model of a material: material is considered as an assembly of discrete elements

In DEM, the motions of each element are described by a couple of equations relating the translational and rotational motions of each element to the resulting force ($F^R{}_i$) and the resulting moment ($M^R{}_i$) acting on that element in a global coordinate system[14] (see Figure 3 (a)). By considering each element as a sphere, the governing equations for element i with mass m_i, position vector r_i and moment of inertia I_i can be written as follows:

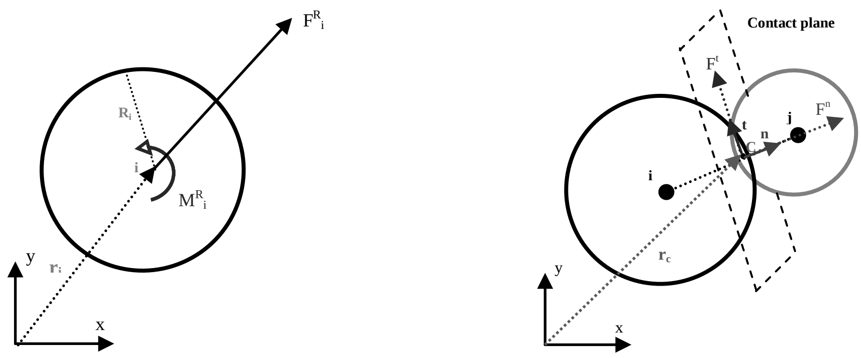
$$F^R{}_i = m_i \ddot{r}_i \quad (6)$$

$$M^R{}_i = I_i \dot{\omega}_i \quad (7)$$

where $\ddot{r}_i$ and $\dot{\omega}_i$ are the translational and rotational acceleration of element i, respectively. The resulting force acting on element i can be expressed by Equation 8:

$$F^R{}_i = \sum F_{ij} + F_i^g \quad (8)$$

where F_{ij} represents the contact force acting on element i by particle j and F_i^g is the body (gravitational) force. The contact force is generally decomposed into a normal component (F^n), which acts normal to the contact plane (tangential plane), and an tangential component (F^t), which acts in the contact plane (see Figure 3 (b)).



(a) (b)

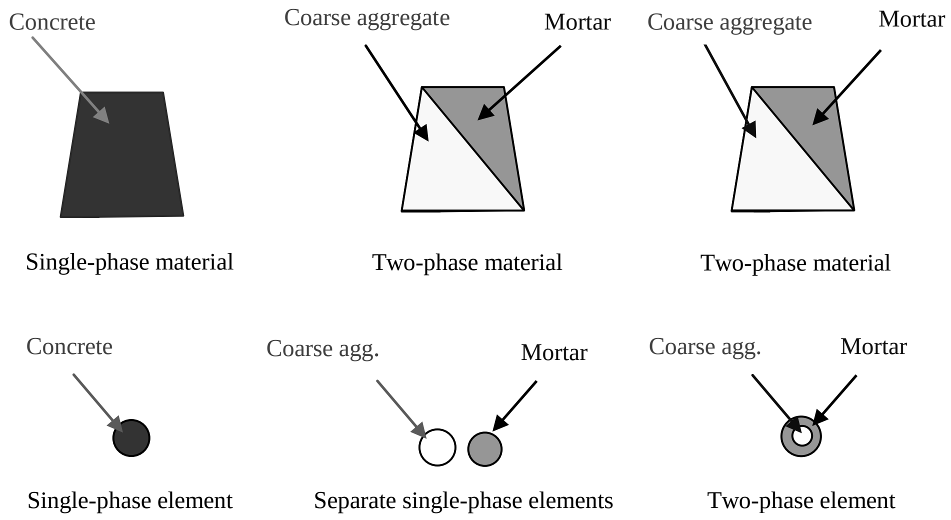
Figure 3 — Characterization of an element in the 2D global coordinate system. a) $F^R_{i,}$ $M^R_{i,}$ R_i and r_i stand for the resulting force and resulting moment acting on element i, radius of element i and position vector of element i, respectively. b) C represents the contact point between two particles while F^n and F^t stand for the normal and tangential components of contact force, respectively. In this figure r_c, n and t are the position vector of the contact point C, unit vector in normal and tangential directions, respectively.

The discrete element models that are available for the flow analysis of a concrete mixture can be divided into three main sub groups as shown in Figure 4.

- Single-phase element model, (Figure 4(a)). The mixture is considered to be a single phase material, represented by the assembly of single-phase elements [15].

- Separate single-phase element model, (Figure 4(b)). The mixture is divided into a mortar phase and a coarse aggregate phase, represented by a combination of separate-single phase elements viz. mortar and coarse aggregate [6, 16].

- Two-phase element model, (Figure 4(c)). The mixture is divided into a mortar phase and a coarse aggregate phase, represented by the assembly of the two-phase elements consisting of the inner hard core coarse aggregate covered with a layer of the mortar [7].



(a) (b) (c)

Figure 4 — The discrete element models for a concrete mixture: (a) single-phase element model; (b) separate single-phase element model; (c) two-phase element model.

In this study, a mixture is considered to be built up of two-phase elements consisting of an aggregate grain which is covered by a layer of paste. Based on the force-displacement law, which is proposed by the authors[17], the inter-element interaction in normal direction can be expressed as shown in Figure 5.

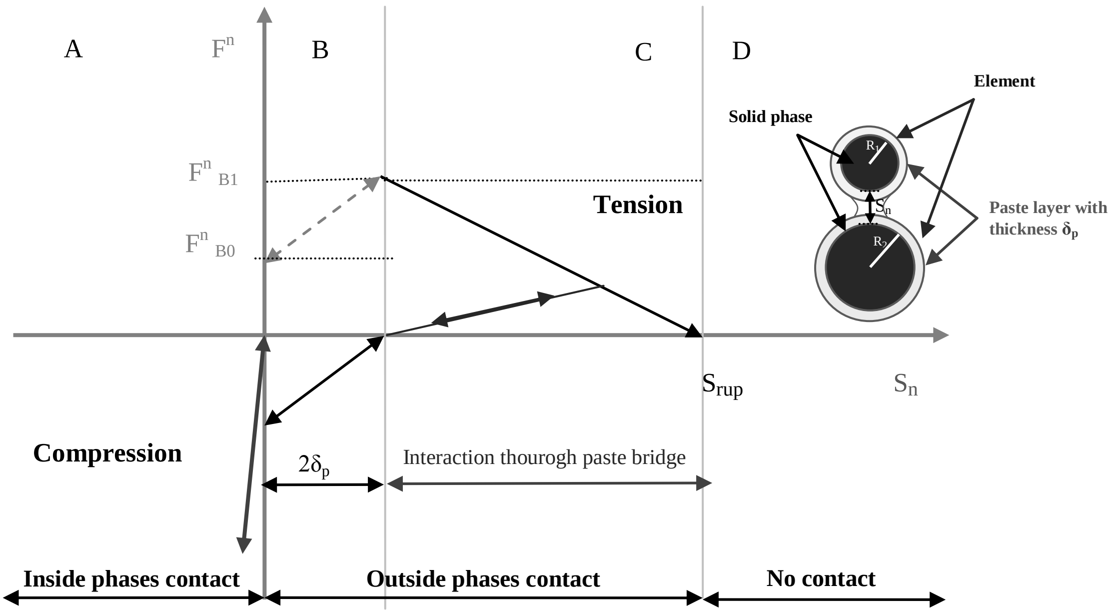


Figure 5 — The interaction force (F^n) - distance (S_n) plot between two discrete elements in normal direction. δ_p and S_{rup} are the thickness of the paste layer and rupture distance, respectively.

Based on this model, the inter-element interaction can be generally divided into three different zones. In zone A, in which the inter-particle distance S_n <0, the inner phases of elements are in direct contact. In zone B, in which the inter-particle distance varies between zero and the sum of the two paste layer thicknesses around each particle $0 < S_n < 2\delta_p$, the interaction happens through contact between paste layers. In zone C, with $2\delta_p \leq S_n < S_{rup}$, the cohesion force due to the presence of the paste bridge decreases by gradually increasing the inter-particle distance. In zone D, with $S_n \geq S_{rup}$, two particles are completely separated and there is no interaction between them anymore. δ_p is equal to δ_{pex} which can be calculated from the mix composition (Equation 5). The other parameters, i.e. F^n_{B0}, F^n_{B1}, which depend on the size of particles and paste consistency, can be obtained from the force-distance formula which has been proposed by the authors before [5]. In tangential direction the elastic-plastic behavior is considered where the elastic behavior is restricted by the Coulomb criterion ($|F^t_{max}| = \mu|F^n|$) [18]. μ (frictional coefficient) is considered equal to 0.7 and 0.5 for inside phases contact and outside phases contact, respectively.

MIX COMPOSITION

The granular material, which is used in this study, consists of river aggregate particles ranging between 1.4 to 1.7 with specific density (ρ_s) of 2.56 gr/cm^3 and a bulk density (ρ_b) of 1.69 gr/cm^3. The volume fraction of the excess paste (V_{pex}) is kept constant 24% (see Table 1). Four paste mixtures are prepared with Portland cement CEM I 52.5 (ρ_s = 3.15 gr/cm^3), limestone powder (ρs= 2.64 gr/cm^3) and superplasticizer. Except for the amount of superplasticizer, the volume fractions of the other ingredients in the paste mixes were kept constant. The volumetric water to cement ratio was of 1.13 (see Table 2).

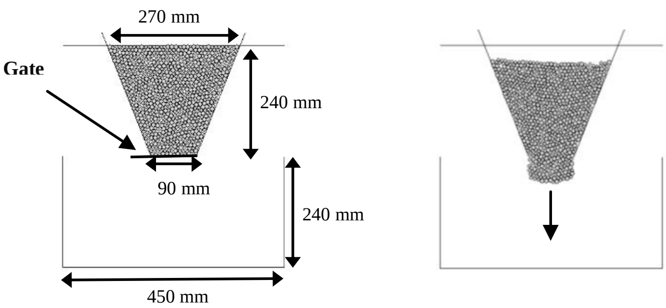
Table 1— Mix proportions of one liter sample.

Mix type	Excess paste volume fraction V_{pex} (%)	Void paste volume fraction V_{pv} (%)	Aggregate volume fraction V_s (%)	Calculated average thickness of paste layer δ_{pex} (μm)	Calculated number of aggregates $\sum N_i$
A	24	26	50	105	26.4E+04

Table 2 — Specifications of the paste phase. Cs stands for the characteristic stress of the pastes.

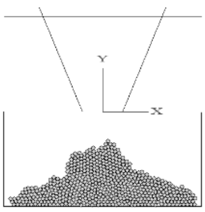
Ingredients	Cement I 52.5	Limestone powder	Water	W/C	
				V/V	m/m
Volume proportion	0.365	0.214	0.413	1.13	0.36
Paste N.	N1	N2	N3	N4	
Superplasticizer [%]	0.71	0.87	0.98	1.26	
Cs (Pa)	37	29	22	11	

It should be mentioned that the consistency of the paste is characterized by the characteristic stress (Cs) which can be obtained from the results of a controlled deformation tensile test [5]. Cs is selected in a way that mixtures can flow under their own weight and fill the mold without applying any external energy. Self-compactability of a mixture is evaluated based on the simulation results of a V funnel shape container test which is proposed by the authors [5]. First a V funnel shape container is filled by the mixture and then the gate at the bottom of the container is opened and the flow behavior of mixture is recorded (see Figure 6). The mixture, which can completely flow out of the container under its own weight, is considered as a self-compacting mixture. The simulation results are presented in Figure 7.

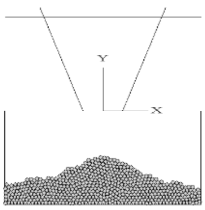


(a) (b)

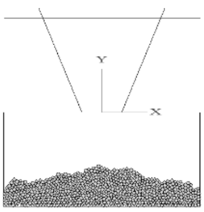
Figure 6 — Evaluation of self-compactability of a mixture based on the flow behavior of a mixture after opening the gate of apparatus (simulations); a) gate is closed and container filled by the mixture; b) gate is opened and mixture starts flowing.



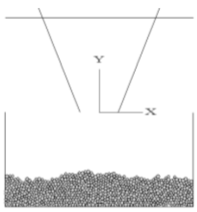
a) A-N1:Cs= 37 Pa



b) A-N2:Cs= 29 Pa



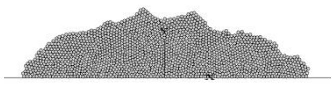
c) A-N3:Cs= 22 Pa



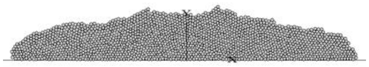
d) A-N4:Cs= 11 Pa

Figure 7 — Simulation results of behavior of the mixtures after opening the gate of V funnel shape container.

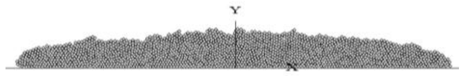
a) A-N1: Cs= 37 Pa



b) A-N2: Cs= 29 Pa



c) A-N3: Cs= 22 Pa



d) A-N4: Cs= 11 Pa

Figure 8 — Simulation results of the slump flow test.

EVALUATION TEST

The macroscopic behavior of a mixture is evaluated by the slump flow test [19]. First the cone is filled in a continuous manner without any compaction. Next, the cone mold is lifted vertically upward and deformation capacity of each mixture is characterized by two quantities, relative spread D/Do and relative slump Hs/Ho. These factors are calculated using the result of the spread diameter (D) and slump (Hs) at ceasing of the flow after removing the cone. The mean value of two perpendicular final spread diameters is considered as a spread diameter (D). The visualized simulations are shown in Figure 8. The experimental results and simulations are compared in Figures 9 and 10. As it is shown simulations are in good agreements with the experimental results.

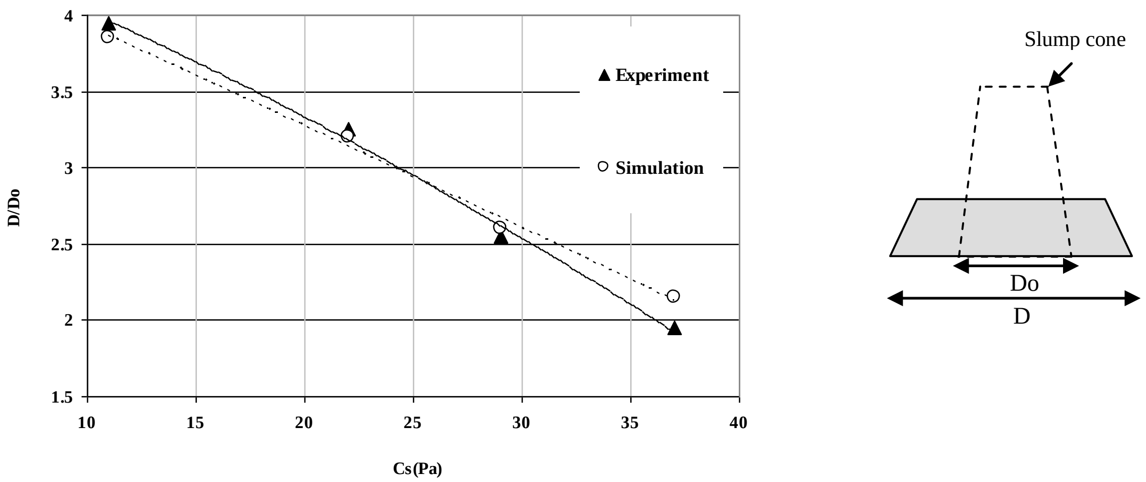


Figure 9 — Relative spread diameter D/Do vs. characteristic stress of the paste Cs. D stands for the spread diameter while Do= 200 mm is the slump cone bottom diameter.

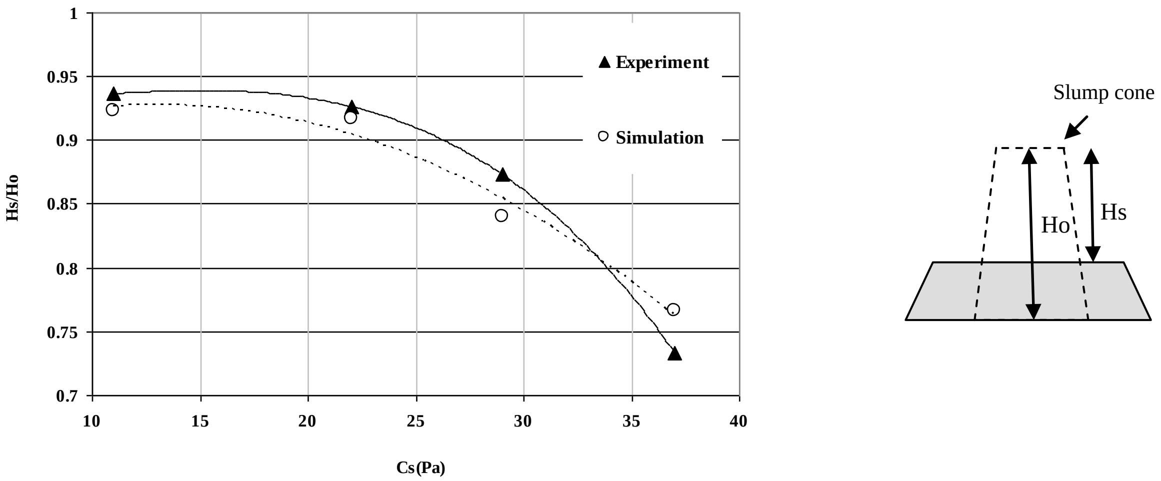


Figure 10 — Relative slump Hs/Ho vs. characteristic stress of the paste Cs. Hs stand for the slump value while Ho = 300 mm is the height of the slump cone.

CONCLUSIONS

In this paper the DEM simulation of the macroscopic behavior of a self-compacting mixture is discussed. The Particle Flow Code 2D (PFC2D) was used as a basic program for the flow analysis of the mixtures. Simulations were carried out based on the two main assumptions:

A) The mixture is a two-phase system and it is composed of two-phase elements, i.e. a solid particle (sphere) covered with a layer of paste.

B) The elements interact with each other during the flow according to the interaction law which was proposed by the authors before.

The approach showed to be very promising in the attempt to predict the flow behavior of a low poly size mixture based on the mix composition. The simulations were in a good agreement with experiments and confirmed the correlation between the paste consistency and macroscopic behavior of the whole system based on the excess paste theory.

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