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Mesoscale modelling of concrete for static and dynamic response analysis Part 1: model development and implementation

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Abstract. Concrete is a heterogeneous material exhibiting quasi-brittle behaviour. While homogenization of concrete is commonly accepted in general engineering applications, a detailed description of the material heterogeneity using a mesoscale model becomes desirable and even necessary for problems where drastic spatial and time variation of the stress and strain is involved, for example in the analysis of local damages under impact, shock or blast load. A mesoscale model can also assist in an investigation into the underlying mechanisms affecting the bulk material behaviour under various stress conditions. Extending from existing mesoscale model studies, where use is often made of specialized codes with limited capability in the material description and numerical solutions, this paper presents a mesoscale computational model developed under a general-purpose finite element environment. The aim is to facilitate the utilization of sophisticated material descriptions (e.g., pressure and rate dependency) and advanced numerical solvers to suit a broad range of applications, including high impulsive dynamic analysis. The whole procedure encompasses a module for the generation of concrete mesoscale structure; a process for the generation of the FE mesh, considering two alternative schemes for the interface transition zone (ITZ); and the nonlinear analysis of the mesoscale FE model with an explicit time integration approach. The development of the model and various associated computational considerations are discussed in this paper (Part 1). Further numerical studies using the mesoscale model for both quasi-static and dynamic loadings will be presented in the companion paper (Part 2).

Keywords: concrete; multi-phase material; material heterogeneity; mesoscale model; nonlinear analysis; explicit time integration.

1. Introduction

Concrete is the most widely used construction material. Due to its multi-phase composition and the quasi-brittle mechanical behaviour, modelling of concrete for structural engineering analysis has been a classical challenge for several decades. Some more recent experimental and numerical studies have focused on the confinement effect, multi-axial loading, softening and dynamic behaviour of the material (e.g., Attaerd and Setunge 1996, Imran and Pantazopoulou 1996,

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Martinez-Rueda and Elnashai 1997, Breitenbucher and Ibuk 2006, Nemecek and Brittnar 2004, Tu and Lu 2009).

An analysis involving the nonlinear response of concrete is often carried out numerically. In a numerical model, the mechanical behaviour of concrete may be described on different physical scales, ranging from homogenised continuum to a microscopic description where the particulates in the cement paste may be explicitly modelled (Emery *et al.* 2007). The selection of an appropriate level of modelling for concrete depends on the scale of observation, characteristics of response, degree of accuracy sought, as well as an affordable computational cost (e.g., Lu 2009).

Generally speaking, modelling of concrete in macroscale with homogenized material properties is computationally economical, and can be suited for a wide range of applications (e.g., Shugar *et al.* 1992, Riedel *et al.* 1999, Malvar *et al.* 1997, Tu and Lu 2009). Because the constitutive laws in such models are derived from the nominal stress-strain response of standard material specimens whose sizes are at least 3-4 times of the largest aggregates in the composite, the applicability of the macroscopic model are generally limited to problems in which the global response is of primary interest in the analysis. Modelling of concrete in mesoscale, on the other hand, permits a direct description of the material heterogeneity and hence allows for a realistic prediction of the development of damage within the multi-phase material. Hence, such a model can be applied to assist in investigating the bulk material behaviour of concrete in a variety of complex stress conditions, and may also be used to analyze the concrete response involving drastic spatial and time variations of stress and strain.

For the mesoscale modelling of concrete, two main alternative approaches have been employed in the literature, namely the lattice models (Schlangen and van Mier 1992, Lilliu and van Mier 2003, Cusatis *et al.* 2003a, b, Leite *et al.* 2004, Nagai *et al.* 2005) and the continuum based FE models (Huet 1993, Sadouki and Wittmann 1998, Wang *et al.* 1999, Kwan *et al.* 1999, Eckardt *et al.* 2004, Tregger *et al.* 2007). In addition, the use of discrete element method (DEM) has also been studied (e.g., Shui *et al.* 2008). A key issue associated with the lattice models and the DEM is the difficulty in determining the equivalent model parameters. The determination of the modelling parameters in a continuum based FE model, on the other hand, is relatively straightforward.

A number of studies on the mesoscale modelling of concrete using a continuum FE model can be found in the existing literature. Wang *et al.* (1999) used the take-and-place procedure to generate the random aggregate structure in 2D and developed a scheme using the advancing front algorithm for the creation of the FE mesh. In the model, the interface transition zone (ITZ) was represented by a four-noded zero-thickness interface element. The model was applied to simulate a simple case of concrete under uniaxial tension. The overall results appear to be realistic, however the predicted tensile strength was less satisfactory. Eckardt *et al.* (2004) presented a similar mesoscale modelling procedure, but disregarded the ITZ and instead considered a rigid bond at the mortar-aggregate interface. Similar treatment of the interface was also adopted in a study by Wriggers and Moftah (2006). De Schutter and Taerwe (1993) described a divide-and-fill strategy for the generation of the concrete mesoscopic structure. Leite *et al.* (2004) developed a stochastic-heuristic algorithm for an improved generation of the three-dimensional concrete mesoscale structure. van Mier and van Vliet (2003) presented the so-called random particle drop method to deal with a higher aggregate volume fraction.

Despite the above mentioned accomplishments, extension of these works to more general applications has been largely hindered by the fact that most of the proposed procedures are implemented in dedicated programs, where there is usually a limited choice concerning the material constitutive models while the capability in handling complex loading conditions is often lacked.

Consequently, it has been difficult to conduct systematic investigations into the concrete failure mechanisms under various loading conditions using such a mesoscale model.

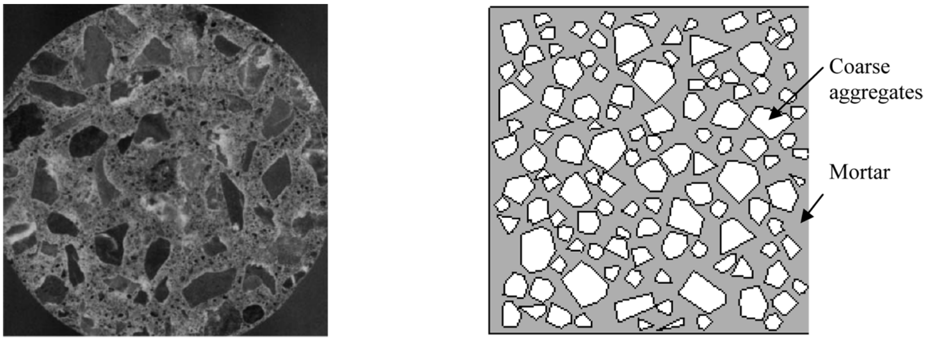
This paper aims to extend the mesoscale modelling framework to analysis involving complex stress-strain and load conditions, including dynamic loading. To this end, the development of the mesoscale model, currently limited to 2D, is oriented towards implementation in a general purpose finite element environment. The complete procedure consists of three main stages, namely, generation of the concrete mesoscopic structure, generation of the mesoscale FE mesh, and FE nonlinear analysis. The paper is organized along the line of the above three aspects, with brief descriptions of the relevant background theories and elaborations of important computational considerations. In particular, two alternative approaches to modelling the ITZ, namely a cohesive interface model and an equivalent layer of solid elements model, are discussed in detail and the corresponding modelling effects are examined. In view of the highly localized nonlinearity in a mesoscale model analysis, an explicit time integration scheme is adopted for quasi-static as well as dynamic analyses. Some associated numerical issues are scrutinized and appropriate counter measures are explored. It should be mentioned that although ANSYS codes are employed to carry out the finite element analysis in the present study, the modelling procedure and essential numerical considerations are applicable with many other general-purpose finite element programmes as well.

Numerical studies using the mesoscale model on the static and dynamic behaviour of concrete will be presented in the companion paper (Lu and Tu 2011).

2. Generation of concrete mesoscopic structure and FE mesh

At the mesoscopic level, concrete can be regarded as being composed of three distinct constituents (phases), namely, coarse aggregate, mortar matrix and interfacial transition zone (ITZ). Fig. 1(a) shows a typical section view of the concrete mesoscopic structure from a physical sample (Grote *et al.* 2001), while a numerically generated model, which will be discussed later, is depicted in Fig. 1(b).

In the present study, the generation of such a complex 2D mesoscopic geometric structure is carried out using Matlab. The geometric information about the aggregates (shape, size, location) and mortar areas obtained in Matlab is written into a macro command file, which is then imported into a mesh generator, herein using ANSYS pre-processor, for the generation of the FE mesh.



(a) Physical sample (after Crote *et al.* 2001) (b) Numerically generated model (not to match with (a))

Fig. 1 Typical cross-section view of concrete mesoscopic geometry

2.1 Generation of coarse aggregates

The generation of aggregates to resemble the random sizes, shapes and spatial distribution in actual concrete is a complicated process. In order to be realistic, a set of physical requirements governing the particulate packing should be satisfied. Once the aggregate structure is formed, the mortar matrix can be generated readily to fill up the space not occupied by the aggregate particles.

In normal concrete, the coarse aggregates are generally defined to consist of particles having a nominal size greater than 4.75 mm (Wriggers and Moftah 2006), and they occupy around 40-50% of the mixture volume. In a 2D model, the volumetric proportion is represented by the area ratio. Actual aggregates may appear in different shapes depending on their source of origin; the naturally formed gravels have a rounded shape whilst crushed stone aggregates have an angular or polygon shape. In the present study, we shall consider mainly the polygon-shaped aggregates. Other special shapes, such as round or elliptical, are relatively simple to generate, and they may also be approximated by polygons with specially chosen shape parameters.

The aggregate size distribution is commonly described using Fuller Curve

$$P(d) = 100.0 \times (d/d_{\max})^n \tag{1}$$

where P is the volume percentage of aggregates below size d, $d_{\max}$ is the maximum size of the aggregate particle. The exponent n generally takes a value in the range of 0.45-0.70 (Wriggers and Moftah 2006). With Eq. (1), the area ratio of aggregates in a given size range can be calculated.

In the numerical simulation, the grading curve expressed in Eq. (1) can be descretized into a certain number (denoted by $i_{\max}$) of segments, each covering a size range of $[d_i, d_{i+1}]$. Thus the amount (area in 2D) of aggregates within each grading segment is

$$A_{a,i} = \frac{P(d_{i+1}) - P(d_i)}{P(d_{\max}) - P(d_{\min})} \times A_a \tag{2}$$

where A_a is the total amount (area) of aggregates in concrete.

Wang *et al*. (1999) presented a comprehensive procedure using a commonly adopted take-and-place method to generate the random geometric structure of aggregates. The basic idea of the take-and-place method is to create the aggregates in concrete in a repeated manner, one at a time, until the target amount of aggregates is fulfilled. The “take” process generates an individual aggregate in accordance with the random size and shape descriptions, in the local coordinate system. The “place” process subsequently positions the aggregate into the predefined concrete area in a random manner, subjected to the prescribed physical constraints.

The above methodology is also adopted in the present study. The procedure is summarized in a flowchart shown in Fig. 2, which is programmed in the present study using MATLAB. After the total amount of aggregates, aggregate size range, grading segments, and aggregate shape parameters are specified, the take and place process is executed in a sequential manner, starting with the largest aggregate size group [d_1, d_2] (for easy packing), and carrying on until the smallest size group is completed. Once an aggregate, A_{ij}, is generated, it is immediately placed into the concrete area by aligning the local polar origin of A_{ij} with a randomly chosen position in the concrete. For the placement to be valid, four physical conditions have to be satisfied simultaneously, namely, a) the aggregate must wholely be within the concrete area, b) there is no overlapping, and c) no intersection between any two aggregates, and d) there is a minimum space between any two

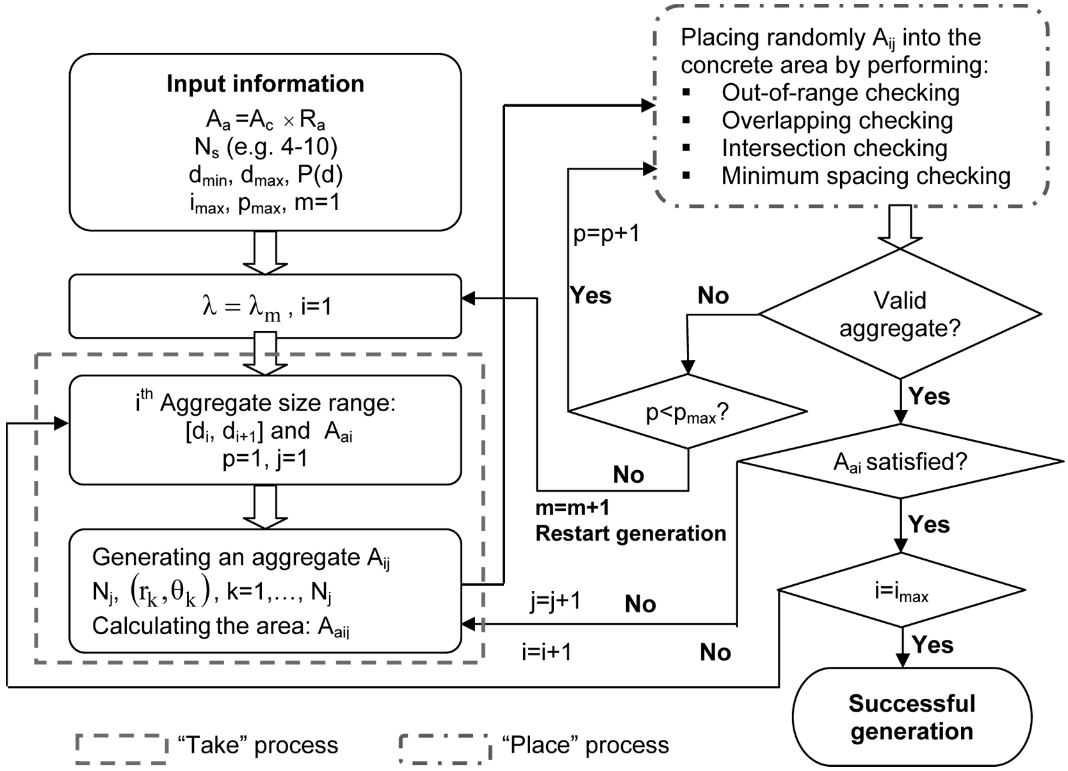


Fig. 2 Flowchart of generating random aggregate structure using take-and-place method

aggregates. The minimum space requirement is aimed to represent the phenomenon that each aggregate particle is coated with a mortar film having a certain thickness.

It is worth pointing out that it is neither economical nor necessary to check each newly placed aggregate against all existing aggregates for overlapping and intersection. Such checking may be confined to a local region surrounding the new aggregate. In the present study the checking region is defined by a diameter equal to four times the largest aggregate, which proves to be sufficient.

If a failure occurs in any of the above checking procedures, the place process is repeated for the same aggregate with another randomly selected alignment position. If a successful placement cannot be achieved after a given number of trials, the generation process is terminated, and a totally new round of generation will be started using a reduced gap size. A typical execution of the above procedure to achieve a successful outcome will take just a few minutes of computing time using a duo-core, 2.7 GHz and 3.2 GB-RAM PC.

2.2 Generation of FE mesh

To mesh the mesoscopic structure of concrete properly, the aggregate polygons should be regarded as the physical boundaries for the surrounding mortar material in the FE model, and different material parts should maintain continuity at their interfaces. A meshing algorithm capable of dealing with the large number of internal boundaries of different shapes and sizes as in the concrete mesoscale structure is very complex and an in-house development of a program for such a task can be costly. As a matter of fact, some general-purpose commercial FE programs have already been equipped with such a meshing capability. In the present study, we employ the pre-processor in ANSYS to mesh the mesoscale FE model of concrete. The procedure is detailed in what follows.

After the generation of the mesoscopic geometric structure as described in Section 2.1, the data is fed into the meshing processor. The concrete domain A_c and the areas representing all the aggregates A_a^i are then created. The areas that are not taken by the aggregates belong to the mortar material, denoted by A_m. A_m is actually a complex multi-connectivity region. In the ANSYS pre-processor, A_m can be generated by applying the "overlapping" Boolean operation between all A_a^i and the entire concrete area A_c.

Meshing of the aggregate areas A_a^i and the mortar area A_m is performed one after the other using their respective material properties. It is important to note that a correct identification of the area numbers associated with A_m and A_a^i needs to be made prior to the meshing operation. This is to ensure that the mortar and aggregate parts are effectively separated and the mesoscale structure is well preserved in the FE model.

The above-generated mesh will automatically have shared nodes at the interface between the two materials. If the interfacial transition zone (ITZ) surrounding the aggregates is to be modelled explicitly, for example by zero-thickness interface elements such as the Goodman model (Kwan *et al.* 1999), a duplicate set of nodes will be required at the interface locations. An alternative way of modelling the ITZ is to use a thin layer of solid elements having grossly equivalent properties as the ITZ. This approach avoids the use of the zero-length elements and hence does not require a

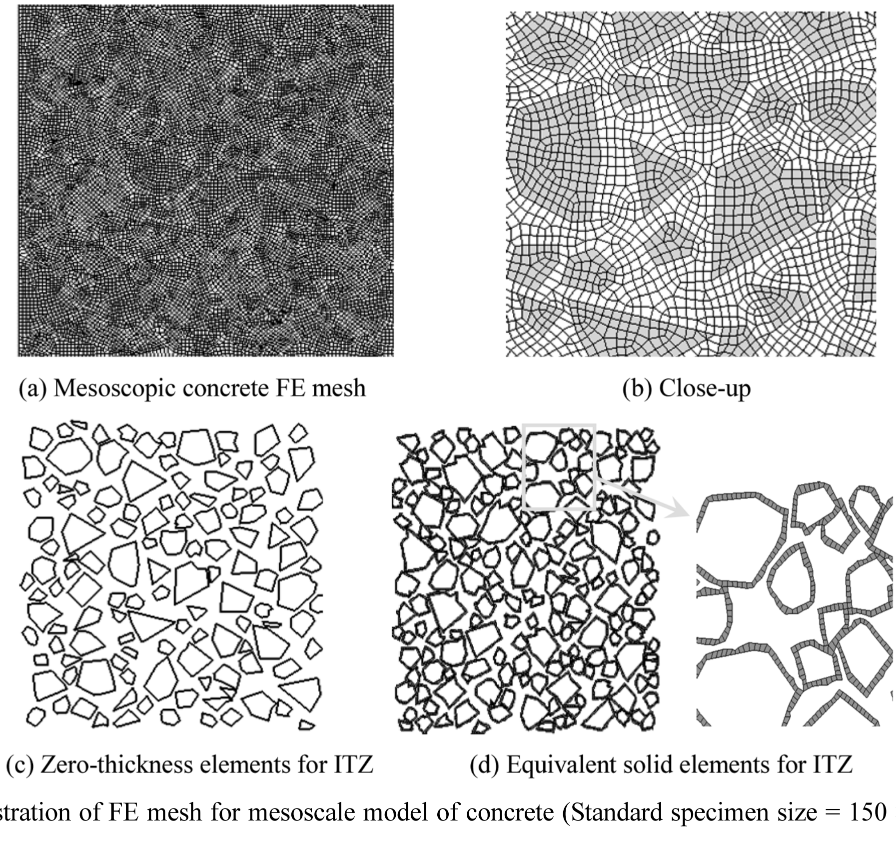


Fig. 3 Illustration of FE mesh for mesoscale model of concrete (Standard specimen size = 150 × 150 mm)

duplicate set of nodes at the interface.

A more detailed description of the two different ITZ modelling approaches and a comparison of their performances will be given in later sections. Fig. 3 illustrates a typical FE mesh of the mesoscopic structure of a concrete cube specimen, including the two different representations of the ITZ.

The numerical nonlinear analysis in this study is performed using LS-DYNA (2007), which is a transient FE analysis program and is suitable for dynamic as well as static analysis. It should be pointed out that a similar procedure can be applied when another general purpose FE solver is employed for the nonlinear FE calculations.

In the next section, a scheme of using the explicit time integration approach for solving the highly nonlinear response problem associated with the mesoscale concrete model will be presented and discussed.

3. Analysis of highly nonlinear static problems using explicit time integration approach

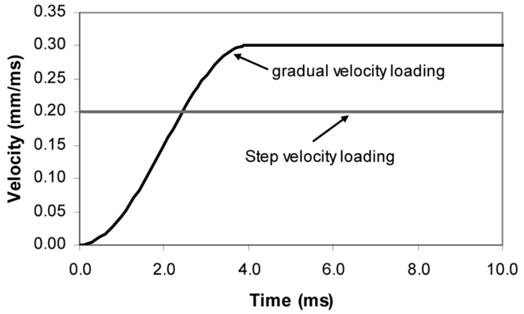
A mesoscale model of concrete may be used to investigate the underlying mechanisms governing the behaviour of concrete material under a variety of loading conditions. However, even under a quasi-static uniaxial compression or tension condition, the response within the mesoscale structure of the material can be very complex due to the involvement of localized deformations associated with fracture. As loading continues a large number of microcracks will develop in the mortar and ITZ, followed by the formation of a few macrocracks due to the coalescence of microcracks. These macrocracks can propagate in the concrete in an uncontrollable or unstable manner, leading to the stress softening of the material as observed in physical experiments.

In the mesoscale model, the process of fracture initiation and coalescence will manifest as localized severe nonlinearity and material degradation, and this can create considerable numerical difficulties in achieving a converged solution if an iterative nonlinear solution approach is adopted. For this reason, and in view of an accommodation for dynamic analysis, an explicit time integration approach (hereafter referred to as ETIA) is adopted as the solution engine. Convergence can generally be ensured with the ETIA by considering an appropriate stable time step. A successful implementation of such a strategy for application in a quasi-static setting requires several important considerations; chiefly the choice of loading history, configuration of the hourglass control, and mass scaling. These will be elaborated in the subsections that follow.

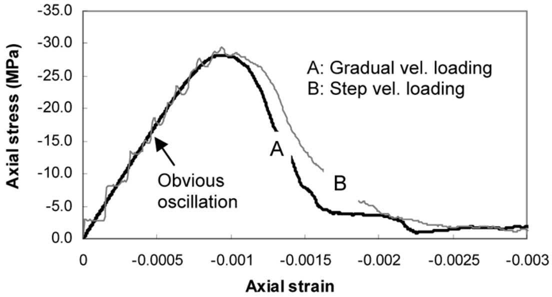
3.1 Configuration of loading history

The ETIA essentially solves a dynamic equilibrium equation set at each incremental time step. When this approach is employed to perform a quasi-static analysis, the loading scheme should be carefully specified so that the inertia effect becomes negligible. A rule of thumb for checking the adequacy of loading is that the kinetic energy of the whole model is sufficiently lower than the internal energy, preferably below 5% (Pan *et al*. 2006). In addition, the time for the force to rise from zero to the expected magnitude should be long enough (say 10 times) as compared to the fundamental period of the system.

In the present study, a displacement controlled loading scheme by imposing a velocity boundary



(a) Two different velocity loading patterns



(b) Simulated stress-strain curves

Fig. 4 Two different loading patterns and the resulting stress-strain responses

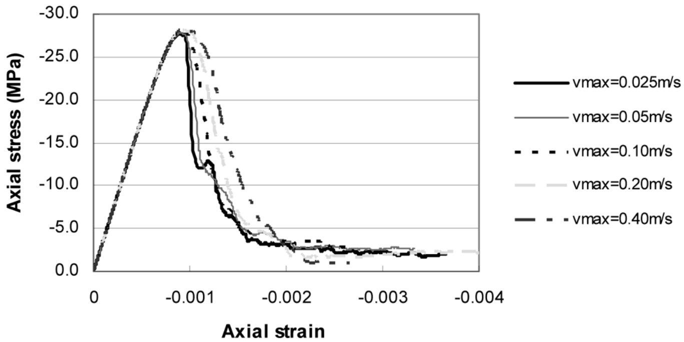
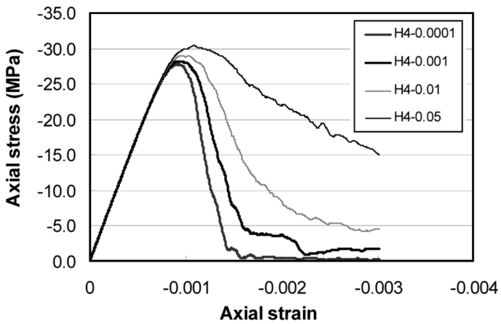


Fig. 5 Stress-strain responses obtained using different loading velocities

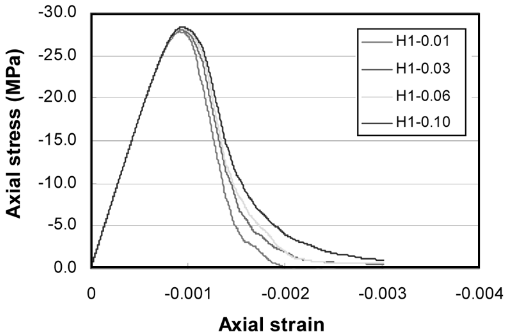
condition is used to load the concrete specimen. Such a loading scheme allows for the realization of the complete response history of the specimen, including the nonlinear strength degradation (softening) phase. To minimize the spurious oscillations, a gradually increased velocity history, as opposed to a step increase pattern, is adopted, as shown in Fig. 4. Controlling parameters that need to be specified include the rise time and the cap velocity. Fig. 5 compares the computed stress-strain responses under a quasi-static compression when five different loading velocities are used in the simulation. The results tend to become stable when the cap velocity is reduced, in this case to an order of 0.05 m/s. At this juncture, it is worth mentioning that some special numerical schemes, such as a dynamic relaxation method (e.g., Rericha 1989), may be incorporated to achieve a more efficient explicit time integration computation in solving static problems.

3.2 Pertinent numerical considerations

In an explicit FE calculation, the element formulation with a single integration point is usually used to control the computational cost. The use of this type of elements also helps to avoid the numerical problems that could happen to fully-integrated elements in case of large deformations, for instance shear locking and solution instability. However, such elements can be susceptible to the problem arising from the so-called “hourglass” modes. The occurrence of these anomalous modes is due to the one-point integration scheme, such that when the diagonally opposite nodes have



(a) Stiffness-based hourglass control



(b) Viscosity-based hourglass control

Fig. 6 Effects of hourglass controls with different schemes

identical velocities, the algorithm will return a false zero strain and stress.

In order to eliminate these modes while maintaining the actual global response, an artificial hourglass-resisting force is usually applied to the elemental nodes. Typically, two different types of algorithms are available for the hourglass control; one based on the stiffness and the other based on viscosity formulations. An hourglass coefficient (Q_{hg}) needs to be specified. Different choices of Q_{hg} can affect the simulation results significantly if the development of the hourglass modes becomes severe. A stiffness-based hourglass control scheme is generally recommended for the analysis of problems under slow loadings (e.g., quasi-static loading), while a viscosity-based scheme may be more appropriate for relatively fast loading scenarios (LS-DYNA 2007). For the mesoscale analysis of concrete in the present study, trial analysis tends to show that Q_{hg} has little effect on the predicted concrete strength, but has sensible effect on the softening response, such that the calculated response tends to become more ductile as Q_{hg} increases.

Fig. 6(a) shows a comparison of the stress-strain results of concrete under uniaxial compression when different choices of Q_{hg} are used in a stiffness-based hourglass control scheme. It can be seen that the elastic response (especially the Young's modulus) is not sensitive to the choice of Q_{hg}. However, the inelastic response, including the peak strength and the descending branch, is affected significantly. With an increase of Q_{hg} the peak strength increases while the softening becomes less steeper (more ductile). It is interesting to note that in all cases the hourglass energy remains within 10% of the peak system internal energy, which would appear to be acceptable in accordance with the general guideline. The numerical simulation results herein suggest that such a recommendation is not necessarily valid in a mesoscale analysis.

For a comparison, Fig. 6(b) shows a set of computed stress-strain curves when a viscosity-based hourglass control is employed. It can be found that the stress-strain response is not as sensitive to different values of Q_{hg} as in the stiffness based scheme. The results are comparable to those using a stiffness-based control with Q_{hg} ranging in 0.001-0.01. In the subsequent numerical investigations, the stiffness based hourglass control with Q_{hg} = 0.001 is used.

Another numerical consideration is the possible use of mass scaling to control the computational cost when using an explicit scheme for a quasi-static analysis. As generally understood, to ensure a stable and accurate solution, the time step in an explicit FE analysis must be small, usually on the order of micro seconds. The mass scaling technique works by introducing artificial mass to the original model to purposely scale up the vibration period of the model, thus increasing the stable time step. This scheme can be particularly effective in an FE analysis in which the time step is governed by a relatively few very small elements, in which case only limited artificial mass needs to be added.

Trial analysis with the mass scaling approach on the current mesoscale concrete model reveals that it is possible to scale up the time step by 2-4 times without affecting adversely the stress-strain relationship of the concrete specimens. However, the detailed fracture pattern may be affected to some extent, particularly for uniaxial tension cases. Therefore, for the numerical investigations in the present study, the mass scaling is not actually applied. Nevertheless, the mass scaling method can be an option in practical applications of mesoscale analysis.

4. Material models and other modelling considerations

4.1 Material models for mortar and coarse aggregate

At the mesoscopic level, damage and the nonlinear behaviour occur primarily in the mortar matrix and along ITZ. Many different constitutive models have been used for modelling the mortar material in a mesoscale concrete analysis. Most of these models adopt a simplified formulation. For example, in the paper by Kwan *et al*. (1999) the biaxial response of mortar was decomposed into two simple uniaxial stress-strain relations, and the accumulation of the material damage was solely based on the failure strains associated with the uniaxial test data.

In the present study, we employ the "Concrete Damage Model" (material #72 in LS-DYNA) to model mortar. This material model is capable of describing the material failure due to tension, shear, as well as compression under various stress conditions, and it also includes pressure and strain-rate dependent features (Malvar *et al*. 1997, 2000). The model has been tested extensively (e.g., Tu and Lu 2009), and is found to be a suitable candidate for quasi-static as well as dynamic applications.

One particular aspect worth highlighting is the treatment of stress softening under tension. In a FE model with a local material description, when an area is subjected to tension, localization will normally occur in a single row of elements. As such, the FE results become mesh dependent if the stress softening law in the material model is an invariant with respect to the element size. This is because the energy required in the actual cracking process is proportional to the area of the fractured surfaces, whereas in a FE model the internal energy due to crack formation is calculated by integrating the stress-strain response over the element volume. To appropriately represent the fracture energy in the FE model, the above two energy terms must be equal, i.e.

$$A_F \times \int_0^{h_c}\left(\int_0^{\varepsilon_{\max}} \sigma d\varepsilon\right)dl = G_f \times A_F \tag{3}$$

where G_f is the fracture energy per unit area, A_F is the area of the fracture surface in an element, and h_c is the nominal dimension of the element in the direction perpendicular to the fracture surface. In a constant stress element the above equation reduces to

$$\int_0^{\varepsilon_{\max}} \sigma d\varepsilon = G_f / h_c \tag{4}$$

Eq. (4) indicates that the stress-strain law must be made dependent on the mesh size in order to achieve a realistic, mesh-independent bulk behaviour of the model.

In the Concrete Damage Model under consideration, the stress-softening related model parameters are automatically adapted to each individual element size in the FE model such that Eq. (4) is satisfied. In addition, the model introduces a user-defined localization width "l_w" to enable another layer of control over the fracture energy, such that in situations where the localization in the FE model may deem to span more than one element width due to particular stress conditions, the fracture energy associated with each element is reduced by a factor of (l_w/h_c) before it is applied in Eq. (4).

The coarse aggregates usually have a significantly higher strength than mortar. In general loading conditions such as quasi-static compression and tension, the aggregates are expected to experience no damage or very limited inelastic response. Therefore, it is reasonable to use a linear elastic material model to model the aggregates. Such a simplified treatment is also adopted in some previous studies (Wriggers and Moftah 2006). For some extreme loading conditions such as shock and blast, damage may occur within the aggregates. Under this circumstance, a nonlinear material model may become necessary and this can be realized within the current mesoscale model in a straightforward manner.

4.2 Interface transition zone (ITZ) modelling

In the multi-phase composition of concrete, ITZ refers to the very thin layer of material immediately surrounding the coarse aggregates. The material in the ITZ is known to be mechanically weaker than the normal mortar, due to factors such as loose compaction and the presence of a high level of void. It is generally recognized that ITZ plays a crucial role in the concrete fracture process; therefore, an adequate representation of the ITZ is an important subject in the mesoscale model.

Past research has found that the thickness associated with the ITZ in concrete is of a similar order as the median size of the cement grains, which is typically in the range of 10-30 micrometer (Garboczi and Bentz 1997). An exact incorporation of such a thin layer of material in the mesoscale FE model is impractical; instead, using zero initial thickness elements (hereafter referred to as interface elements) is deemed to be a rational representation.

Several issues can affect the performance of using zero-thickness elements approach for the ITZ. When such elements are subjected to compression in the thickness direction, cross-penetration of the element nodes could occur, causing unexpected numerical error and even instability in the overall simulation results. Moreover, the general constitutive models (cohesive models) for the interface elements are formulated primarily to model interface fracture, and they may not represent well the shear response and the interaction between shear and compressive stresses. Therefore for the analysis in general stress conditions, more sophisticated interface element models will be required and this is beyond the scope of the present paper.

As an alternative to the zero-thickness interface element model, in the present mesoscale modelling framework we propose to use an equivalent (thin) layer of solid elements to represent the ITZ. This approach can readily avoid the difficulties associated with the interface elements mentioned above, while still retains the essential mechanisms of the ITZ in the loading process. Detailed considerations of the material properties used for the equivalent ITZ elements, and a comparison of the simulation results using the two different ITZ modelling approaches will be presented in Section 5.

When using the equivalent ITZ approach, the equivalent ITZ layer is composed of the elements that immediately surround the aggregates, and will be modelled as a separate part. These ITZ

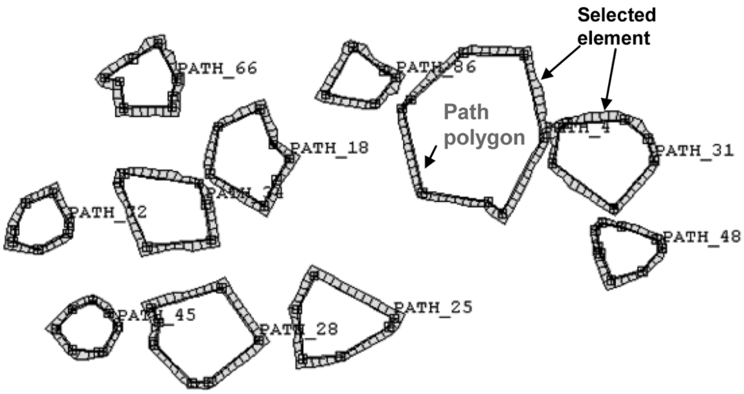


Fig. 7 Illustration of example paths and ITZ elements identified through these paths

elements must be identified from the overall model first. There may be different ways to do this, and a convenient approach is to use a “selecting elements by path” function which is available in ANSYS and other FE pre-processing tools. To pick out elements surrounding an aggregate, the path can be defined effectively by a polygon which is a slightly expanded version of the actual aggregate. Such paths can be conveniently generated during the creation of the aggregates in the take-place procedure. Fig. 7 depicts some example paths and the ITZ elements thus identified.

4.3 Finite element model configuration and mesh gird size

Quadrilateral elements are used in most part of the concrete. Some triangular elements may be required at a few highly irregular locations such as in-between two or more very closely spaced coarse aggregates.

Because the concrete material model used in the present study is restricted to 3D solid elements, the current 2D mesoscale model is analyzed in a thin plate configuration, with a single layer of elements in the out-of-plane direction. To maintain the virtue of a 2D problem, the element thickness is chosen to be equal to the nominal mesh size in the 2D plane so that the characteristic dimension of the elements is identical to that evaluated from the 2D geometry. A 2D plane stress or plane strain condition may be simulated readily by restraining the out-of-plane movement on one side (plane stress) or both sides (plane strain), respectively.

The nominal mesh grid size (element size) is chosen to be about 1.0 mm. This choice is a result of trade-off between the need to adequately mesh all individual phases and the computational cost. A convergence study indicates that such element size generally ensures the mesh convergence as far as the overall behaviour and the characteristic damage patterns are concerned.

5. Comparison and discussion of the two ITZ modelling schemes

As described in Section 4.2, two alternative modelling schemes are considered for modelling ITZ, namely a zero-thickness interface element scheme, and an equivalent layer of solid element scheme. This section provides a comparison between using these two different schemes and discusses their performances.

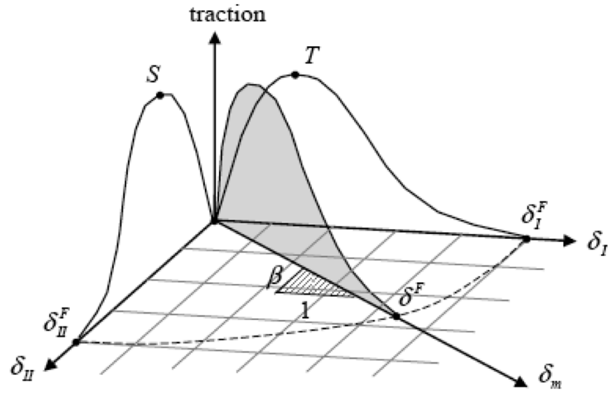


Fig. 8 Illustration of mix-mode constitutive law for cohesive elements (after LS-DYNA 2007)

A cubic concrete specimen of 150 mm is modelled for uniaxial compression and tension. The nominal concrete strength is 30 MPa. Further details about the configuration of the model and other model settings can be found in the companion paper (Lu and Tu 2011). The ITZ properties in association with the cohesive material model are based on a previous study (Kwan *et al.* 1999).

The ITZ material properties are not precisely known in the literature due to the difficulty in conducting reliable experiment on these properties. But it is generally accepted that the ITZ material has a strength about 50% of the mortar strength. This value is adopted herein when the interface (cohesive) element is used. In the equivalent ITZ model, however, considering that the equivalent layer is an equivalent mixture of the real ITZ and the adjacent mortar, it is deemed rational to adopt an averaged strength, i.e., 75% of the mortar strength for the equivalent ITZ.

The cohesive model used here for the interface elements is a typical cohesive model which is suited for modelling the interface failure involving interaction between mode I and mode II fractures (LS-DYNA 2007). This element model considers the irreversible damage and allows for an independent definition of the constitutive relations for different fracture modes of tension and shear. The compression behaviour is treated as elastic and is calculated using a penalty based algorithm similar to that adopted for a general contact model. Fig. 8 shows schematically the constitutive laws used in the cohesive material model. The constitutive laws used for modelling of mode I and mode II fractures are depicted by the curves in the "traction-δ_I" and "traction-δ_{II}" planes, respectively, where δ_I and δ_{II} denote respectively the normal and tangential separation distance. The mode mixity β is defined as $\beta = \delta_{II}/\delta_I$. δ_F is the ultimate mix-mode displacement and is a function of (β, T, S) and the fracture energy associated with model I and II fractures. When the element is subjected to compression, the model implements a penalty algorithm to work out a repulsive force to avoid inter-node penetration. However, it should be pointed out that it is difficult and problematic to determine an appropriate penetration stiffness factor (PSF) to effectively avoid the inter-node penetration. A larger PSF can generally effect to minimize the penetration problem, but it may also cause the corresponding numerical calculation to become unstable.

Fig. 9 compares the simulated stress-strain response under uniaxial compression using respectively the interface element and equivalent element models for the ITZ. It can be immediately observed that the numerical model in which the ITZ is modelled by the interface element fails to produce a realistic compressive response of concrete. On the other hand, the model using the equivalent ITZ

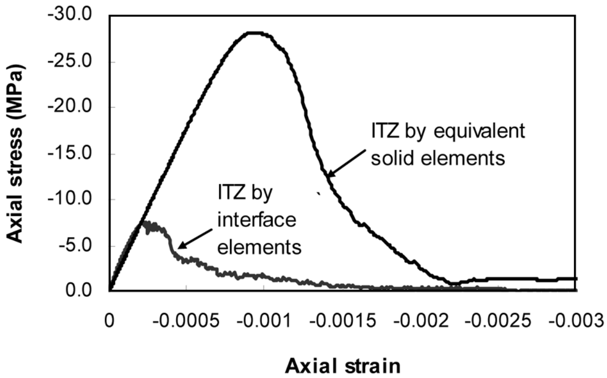


Fig. 9 Uniaxial compressive stress-strain relationships produced by mesoscale concrete model with two different ITZ modelling schemes

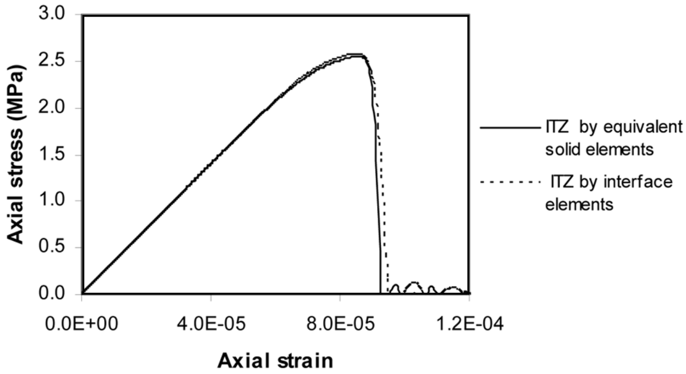


Fig. 10 Uniaxial tensile stress-strain relationships produced by mesoscale model with two different ITZ modelling schemes

scheme shows a superior performance in predicting the compressive stress-strain relationship as well as the peak strength.

The poor performance of using the cohesive interface element may largely be attributable to the inability of this model in representing the shear fracture strength of the ITZ under a compressive stress condition. As generally known, the shear fracture strength of the ITZ in concrete-like materials is strongly dependent on the normal stress at the interface. With the presence of a compressive stress, the shear strength is expected to increase significantly, for example by 2-3 times at a moderate compressive stress level (Nagai *et al*. 2005). Unfortunately, this important mechanism is not well represented in a general cohesive material model as used herein.

It can be expected that the above-mentioned issues with the cohesive model have minor consequence in analyzing concrete under uniaxial tension, as the level of compressive stress in the ITZ would become insignificant. Fig. 10 shows the comparison between the predicted tensile stress-strain curves using cohesive interface element and the equivalent ITZ models. The results agree well. The simulated tension crack pattern with the cohesive interface element for the ITZ is shown in Fig. 11. A single crack across the whole width of the specimen is observed, as expected.

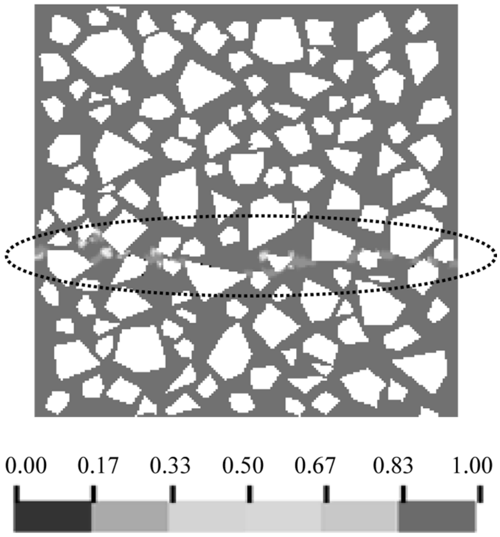


Fig. 11 Simulated fracture pattern of concrete under uniaxial tension using interface elements for ITZ (Note: the colour scale indicates damage with 1.0 being total damage)

6. Conclusions

This paper presents the development of a mesoscale model with the aim to cater to analysis under complex stress-strain and general loading conditions, including dynamic loading. The mesoscale model is currently limited to 2D, but the model framework is not restrictive and can be readily extended to a 3D environment when the generation of 3D mesoscale geometry becomes attainable.

In the proposed framework, the mesoscopic geometric structure of concrete is generated using an established take-and-place algorithm, coded in the present study using MATLAB. The mesoscale geometry data is subsequently taken into a FE meshing processor (ANSYS) to perform the complex FE meshing task. Considerations are given to ensure an adequate meshing of the multi-connectivity concrete domain and identify elements belonging to the 3 different phases for the material property assignment. Advanced nonlinear material models, such as the Concrete Damage Model and the cohesive interface model, can be readily incorporated to model the mortar matrix and the ITZ. To overcome the numerical problems in solving the mesoscale response, which involves highly localized nonlinearity and material softening, an explicit transient analysis approach is adopted for the analysis under quasi-static as well as dynamic loading conditions.

Because of the crucial role the interface transition zone (ITZ) plays in the fracture and failure process of concrete, a dedicated study is carried out to investigate the performance of two alternative modelling approaches for the ITZ, namely the zero-thickness interface element approach and an equivalent layer of solid elements approach. It is found that the interface element approach with a generic cohesive material model appears to be problematic for general applications, especially when compressive stresses are involved.

Detailed implementation examples using the proposed mesoscale model and a numerical investigation into the concrete behaviour under both static and dynamic loading conditions will be presented in the companion paper.

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