Discrete Element Simulation of Brittle Porous Material Failure

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Abstract. The study uses Particle Flow Code (PFC) 2D discrete element software to reproduce the dynamic compressive experiment of foam concrete, a typical brittle porous material, and to calibrate micro-parameters of hardened cement mortar, building a discrete element model of foam concrete. Experimental phenomena and inner mechanisms are further analyzed and studied, leading to conclusions in the deformation characterization, failure mode and failure mechanism of foam concrete specimens under different strain rate loading. The research results indicate that under low strain rate loading, the specimen cracks from inside evenly; the processes from failure to compaction is endoenergetic, resulting in stress plateau phenomenon and even deformation during the experiment. Under high strain rate loading, cracks are generated in an explosive manner at the impacted end, and the specimen on the whole is not damaged evenly. Simulation results basically fit the experiment data. The peak stress curve fitting of concrete foam from under quasi-static conditions to high strain rate is studied, which shows obvious strain rate effect that grows exponentially. By calculating models with different densities, it is found that the compressive strength of foam concrete increases along with the growth of density. Thus, PFC can be used in numerical simulation of dynamic mechanical properties of brittle porous materials.

1. Introduction

Foam concrete is lightweight and good in heat preservation, insulation, fire resistance and impact energy absorption, and is thus widely used in military defense, civil architecture and road construction, etc. Since foam concrete contains a large number of closed pores, the pores deform in different ways under different impact loading conditions, presenting diverse failure modes.

There has been relatively in-depth experimental research of dynamic and static mechanical properties of foam concrete at home and abroad. The influence of foam concrete’s density on fluidity, compressive strength, water absorption and drying shrinkage property have been studied, and dynamic mechanical properties and failure modes under typical strain rate conditions have thus been found,
which point out that the dynamic ultimate compressive strength of foam concrete has a strain rate effect and the stress-strain curve has an obvious stress plateau\(^\text{[1-5]}\). In terms of numerical simulation, previous research mainly simulated the deformation modes, deformation and instability process, and stress unevenness of porous materials like foamed aluminum and foam concrete at different loading speeds through finite element method (FEM)\(^\text{[6-7]}\). Some research simulated the impact of porosity distribution on the failure process of foam concrete through a combination of FEM and random search algorithm \(^\text{[8]}\). Since foam concrete is a brittle porous material, the complex interactions between and nonlinear behaviors of its particles cannot be presented accurately through the FEM approach, and the microscopic failure process of foam concrete under large deformation conditions, such as crack, defect and stress concentration, cannot be simulated. Whereas, the discrete element simulation approach, developed in recent years, bonds and combines the research object in the form of particle sets, endowing particles with micro-parameters of the material itself and setting intergranular contact parameters and modes of action. Discrete element simulation is an effective numerical computation method for studying the structure and motion law of non-continuous particulate matters \(^\text{[9-10]}\), and can be applied in simulating crack growth, damage cumulation and fracture, failure impact and seismic response, etc.

This study conducts numerical modeling of the compression test of foam concrete through discrete element method (DEM), calibrates micro-parameters of foam concrete by applying uniaxial compression test and uniaxial tension test data, and builds foam concrete models as well as SHPB simulator. The stress plateau phenomenon and strain rate effect of foam concrete is also simulated and studied, and compression of foam concrete with different densities analyzed.

2. Discrete Element Simulation and Parameter Calibration of Foam Concrete

2.1. Basic discrete element assumption

Discrete element method forms specific materials by combining generated individual particles in the form of bond. PFC, a typical numerical simulation software for studying particle flow, assumes all generated particles as rigid bodies. Particles contact each other through internal force and moment of force, and overlap each other at the contact point. Thus, the contact can be defined as point contact. The relative displacement between particles follows the force-displacement laws, and is correlated with the contact force. The connecting bond exists at the contact point, and the long-distance interaction can be calculated through applying potential energy function. Since PFC allows large deformation and fracture and detachment of macro structure, and deformation or fracture is caused by translation and rotation of particles, PFC approach is of great advantage in simulating mechanical properties of brittle materials\(^\text{[11-13]}\).

A large proportion of deformation in a physical system is presented as movement along the interface. Deformation is mainly caused by the interaction between particles that act on rigid bodies, instead of by the deformation of individual particles. In discrete element theory, when the internal force reaches equilibrium, the interaction between particles can be regarded as a dynamic process in equilibrium state. Through tracking the movement of each particle, the contact force and displacement of particle sets can be calculated. Assuming the speed and accelerated speed are constant for each time step, the dynamic step length can be described in time steps. By adopting explicit numerical
computational method to simulate non-linear interactions between a large number of particles, excessive storage and iterations are avoided \[14\].

2.2. Selection of contact model

As particles stick to each other through bonded contact, the entity composed of particles can be regarded as brittle materials. The interface of flat-joint model consists of units, and the failure of bonded units will result in local failure of the interface, and the fracture of interfacial bonded contacts lead to cracks. In a flat-joint model, the contact interface of particles is segmented, as shown in Figure 1. When the bonded contact reaches failure conditions, the bonding effect disappears, yet friction still exists between particles. The units can be either bonded or unbonded, and the bonding is linear and elastic. The cracks will not overlap or merge with each other.

2.3. Calibration of micro-parameters and modeling

In PFC, the setting of material parameters is conducted through defining intergranular micro-parameters, i.e. selecting intergranular parameters that ensure the material’s macroscopic mechanical properties are delivered on the whole. Usually, the parameters will be calibrated through typical uniaxial tension and uniaxial compression tests. When a certain set of intergranular micro-parameters are in line with all macro-mechanical properties of the material, the model can be used to simulate the material.

The same elasticity modulus as the macroscopic one is selected for debugging. The specimen’s failure mode is controlled by adjusting the normal to tangential bond strength ratio. The coefficient of friction only works on bonded contact after failure, instead of on the calibration of macroscopic strength \[16\], and is thus set at 0.577 according to existing calibration data.

Through biaxial compression and uniaxial tension tests \[17\]-\[18\], the cement mortar’s elasticity modulus, Poisson’s ratio and compressive strength \(\sigma_c\) are calibrated. As for the calibrated model, Young’s modulus \(E=2.42\) GPa, Poisson’s ratio \(\nu =0.25\), compressive strength \(\sigma_c=91\) Mpa, and tensile strength \(\sigma_t=8.3\) Mpa.

The comparison between calibrated results and reference macro-mechanical parameters of hardened cement mortar in literature is introduced in Table 1. It can be seen that the gap between calibrated results and reference values in literature \[19\] is relatively minor, meaning that the
micro-parameters (Table 2) can be used to represent hardened cement mortar and build foam concrete model.

Table 1. Comparison between simulation results of hardened cement mortar and reference values

| Mechanical property             | Reported value in literature | Simulation result |
|--------------------------------|------------------------------|-------------------|
| Elasticity modulus E (GPa)     | 0.7~2.8                      | 2.42              |
| Poisson’s ratio                | 0.25                         | 0.25              |
| Compressive strength (MPa)     | 15~150                       | 91                |
| Tensile strength (MPa)         | 1.4~7                        | 8.3               |

Table 2. Main micro parameters of discrete element of cement mortar

| Main micro parameter                              | Calibrated result |
|--------------------------------------------------|-------------------|
| Contact modulus (Pa)                              | 25e10             |
| Normal to tangential rigidity ratio               | 3.6               |
| Porosity                                         | 0.1               |
| Minimum particle radius (m)                       | 0.15e-3           |
| Maximum to minimum particle size ratio            | 1.5               |
| Flat-joint model bonding modulus (Pa)             | 2.5e10            |
| Flat-joint model normal to tangential rigidity ratio | 3.6               |
| Flat-joint model compressive strength (Pa)        | 2.2e7             |
| Flat-joint model shear strength (MPa)             | 5e7               |

The foam concrete used in our experiment is relatively simple in composition and structure. It is composed of mortar and holes. A study conducted by Ramamurthy et al. [20] showed that the foam concrete’s density and strength can be influenced by the volume and diameter of pores, instead of the shape of pores. Since shape has no tangible influence on the foam concrete’s compressive strength and failure mode, it is randomly decided in our experiment, instead of being deliberately designed. The final foam concrete’s PFC model has an equivalent density of 1,080 kg/m³, consistent with the foam concrete in reality.

3. Analysis of Compression Failure Test Results of the Foam Concrete

3.1. Dynamic loading results

Figure 2 shows the failure process of foam concrete specimen under a strain rate loading of 500 s⁻¹. Cracks first occur in structural weak areas close to the impacted end and do not stop developing forward until the whole specimen is covered with evenly distributed cracks. Then, the cracks stop developing at four corners of the specimen, yet they still grow at the center (i.e. structural weak area). As loading continues, the specimen’s internal cracks are distributed in the shape of V. A large amount of strain energy is released at the free edge, and crushing begins.
Figure 2. Simulation of the failure process of foam concrete specimen under low strain rate

Figure 3 shows the simulated failure process of foam concrete specimen under a strain rate loading of 1500s⁻¹. Similar to that under low strain rate, cracks first appear on the surface of specimen, close to the impacted end. Then, cracks develop around the impacted end, forming a region with densely distributed cracks. Obvious shear bands occur at structural weak areas, and continue to develop as loading goes on. The cracks, first generated evenly, now develop in an explosive manner, and evident deformation and collapse of the specimen occurs. Droplets and small blocks of the foam concrete start scattering around.
3.2. Strain rate effect of the foam concrete

The discrete element model of foam concrete is simulated under five different strain rate loading. The strain rate of 1500s\(^{-1}\), which is not achieved in experiments, is also simulated, and the peak stress reaches 25MPa, higher than 18MPa under the strain rate of 1050 s\(^{-1}\). Figure 4 shows the fitting curve of peak stress growth in experiments and simulations under different strain rates. An obvious strain rate effect of the foam concrete specimen can be observed, which basically fits the experimental curve. Intermediate strain rate, which is not involved in experiments, is simulated. Under intermediate strain rate, the peak stress value grows along with strain rate in an exponential manner, instead of linearly.

From the perspective of material, since there are a lot of pores and microcracks in the foam concrete, as the strain rate increases, the number of cracks generated due to compression grow, and the accumulated energy increases. Without enough time to consume the energy, stress increases to compromise the growing energy, which explains why higher strain rate leads to higher strength of the foam concrete.

Figure 3. Simulation of the failure process of foam concrete specimen under high strain rate

Figure 4. Relationship between peak stress and strain rate of foam concrete
4. Influence of the Foam Concrete’s Density on Strength

The density level is altered through adjusting the ratio of pores. By adopting the same modeling approach as in the above sections, foam concrete specimens with different densities are obtained. Exert speeds of 0.05m/s, 0.1m/s, and 0.2m/s on the specimen models. It can be found in Figure 5 that the peak stress of foam concrete specimen with a density of 1260kg/m$^3$ is approximately 6.5MPa, while that of the specimen with a higher density at 1350kg/m$^3$ is 14MPa, showing a sharp increase. However, the stress plateau value does not increase, indicating that higher density may lead to higher compressive strength of foam concrete, but has no evident impact on the stress plateau value. So higher density increases the foam concrete’s strength, but does not improve its energy absorption performance. Specimens with different densities show stress-strain curves with different features when compressed, and the peak stress reduces along with loading speed.

![Stress-strain curves at different loading speeds](image)

**Figure 5.** Stress-strain curves at different loading speeds, (a) $\rho=1260$kg/m$^3$ (b) $\rho=1350$kg/m$^3$

5. Conclusions

The study builds a discrete element model of foam concrete based on flat-joint contact and simulates the compressive failure process of foam concrete under different strain rate loading. The numerical simulation results represent the forming and development of cracks during the failure process. A simulation of the foam concrete’s failure process under a strain rate that is not achieved in experiments is conducted, and curve fitting of experimental data is completed. By building foam concrete models with different densities and running simulation tests, the peak stress is obtained. Our main conclusions are as follows:

1. Under low strain rate, cracks are generated evenly inside the foam concrete. The failure-compaction process of holes is endoenergetic, appearing as stress plateau phenomenon in experiments. Under high strain rate, cracks grow in an explosive manner at the impacted end, and the specimen’s failure on the whole is uneven.

2. Simulation of the compression experiment of foam concrete from under quasi-static conditions to high strain rate shows evident strain rate effect, and peak stress grows exponentially.

3. Stress unevenness of the specimen under high strain rate is due to instability and stress concentration caused by pores hindering the propagation of stress wave inside the specimen.

4. Evident strain rate effect exists for foam concrete specimens with different densities. The compressive strength of specimens increase along with density, yet density has no obvious influence
on the stress plateau value. Thus, higher density of foam concrete may increase its strength but does not improve energy absorption performance.

6. References

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