

基于生成对抗网络的硬化浆体孔隙结构三维重构

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摘 要: 基于 X 射线 CT 图像的水泥净浆微观结构的精确三维重构对水泥基材料的性能预测至关重要, 但传统方法难以捕捉复杂的多尺度孔隙结构或计算成本高昂。为解决这些挑战, 本工作提出了一种深度卷积生成对抗网络(DCGAN)架构, 将自动编码器集成用于多尺度特征学习, 并在带梯度惩罚的 Wasserstein 生成对抗网络(WGAN-GP)框架下实现, 以增强训练稳定性。引入孔隙率约束损失函数以确保生成过程中的全局孔隙一致性。该模型基于石灰石煅烧黏土水泥浆体[55%(质量分数)普通硅酸盐水泥, 30%煅烧黏土, 15%石灰石; 水胶比=0.42]在养护龄期为 3、28、90 d 和 180 d 时的微 CT 图像进行训练。利用闵可夫斯基泛函(孔隙率、表面积、欧拉特征)和空间相关函数[两点相关函数(S2)、线路径函数、两点聚类函数和表面相关函数]对重建的三维结构与实验真实微观结构进行验证。结果表明, 所提出的模型在保持与原始微结构孔隙特征一致的同时, 具有较高的结构保真度, 并显著提高了计算效率(提高约 150%)。该方法能够实现高精度的微结构重构, 进而实现更可靠的基于微观结构的水泥基材料性能模拟。

关键词: 硬化浆体; 神经网络; CT 图像; 孔隙结构; 三维重构

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1 Introduction

In recent years, the continuous development of 3D reconstruction methods for porous media has promoted the integrated evolution of image modeling, performance prediction, and multi-scale microstructure analysis. Traditional image reconstruction methods primarily construct 3D structures from single 2D images, emphasizing the restoration of geometric features and fidelity control. Among these, by coupling a generator with an encoder, low-level features can be effectively transmitted to higher-level ones, maintaining structural pore continuity and detail representation capability during the training process. Meanwhile, the discriminator incorporates a multi-scale structural design, enabling the model to focus on both the local details of pores and the overall

topological features during reconstruction, thereby significantly enhancing the overall restoration accuracy of the structure^[1]. Another category of methods emphasizes the statistical matching of structural features. These approaches evaluate consistency between reconstructed volumes and target volumes in terms of phase volume fraction, connectivity, geometric metrics, and other aspects, while also employing mechanical techniques such as phase-field fracture models to validate their reliability. Meanwhile, to enable performance evaluation and material characterization under limited experimental data conditions, statistical equivalence analysis and virtual sample simulation methods are widely adopted to compensate for the insufficiency of experimental data and enhance the practicality of reconstructed structures^[2]. In recent years, deep learning has been

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widely introduced into pore structure reconstruction. By utilizing fully convolutional networks (FCNs) to extract pore information from scanning electron microscope (SEM) images and combining t-SNE dimensionality reduction algorithms to analyze structural features, this approach has revealed the influences of factors such as curing time, aggregate gradation, and water-to-binder ratio on pore evolution^[3]. In the realm of statistical models, two-point and three-point correlation functions (S2, S3) obtained through Monte Carlo sampling techniques can effectively characterize the spatial distribution of complex structures. Researchers have integrated these functions with various classifiers such as Support Vector Machines (SVM), Probabilistic Neural Networks (PNN), and decision trees to achieve intelligent identification and classification of porous media types, significantly enhancing the robustness and generalization capability of reconstruction models^[4]. Generative Adversarial Networks (GANs) have demonstrated outstanding performance in microstructure reconstruction in recent years. A typical strategy involves first generating coarse-grained structures through GANs, then refining microscopic details using autoencoders to achieve multi-scale integrated reconstruction. This method effectively balances morphology and texture, producing high-quality structures that exhibit both macroscopic skeletons and microscopic pore characteristics. Moreover, compared to traditional Morphology-based Joint Quality Assessment (MJQA) methods, it offers higher training efficiency and greater structural diversity, and has been widely applied in pore reconstruction of media such as sandstone and carbonate rocks^[5]. Furthermore, descriptor-based methods can predict the statistical characteristics of 3D structures using only 2D images, overcoming the limitations of 3D image acquisition while maintaining scale consistency and statistical equivalence in the reconstruction results. In terms of evaluation methodologies, studies widely employ two-point correlation functions and the convergence behavior of interface pixel concentration as accuracy criteria to monitor whether the reconstructed structures faithfully

reproduce the features of the original images at both global and detailed levels^[6].

In addition, a multi-scale GAN network (multi-GAN) has been proposed to further extract hierarchical features from images. Utilizing a convolutional pyramid structure, it learns full-scale information from a single 3D image, demonstrating superior generation performance compared to traditional MJQA methods and enabling applications in various media structure reconstruction tasks^[6, 7]. In specific material systems, researchers have integrated micro-CT data with mechanical simulations to reveal the correlations between pore structures and mechanical properties. This approach achieves macro-micro scale bridging through homogenization processing and grayscale distribution analysis of images^[8]. In terms of pore geometric characteristics, researchers employ methods such as the two-point correlation function and Minkowski functionals to extract metrics including volume, specific surface area, and Euler characteristic. These metrics are used to evaluate the storage capacity, connectivity, and percolation properties of the structures^[9, 10]. At the algorithmic level, optimization techniques such as differential evolution have been incorporated into the two-point stochastic optimization (TPSO) framework to enhance the efficiency and accuracy of structural reconstruction^[11]. Regarding evaluation metrics, while the Fréchet Inception Distance (FID) is widely used for assessing the quality of generated samples, its application to pore structures is more appropriately combined with physical characteristics like Minkowski functionals to better align with the requirements of real porous media^[12]. The multi-scale GAN architecture further improves the realism and generalizability of reconstructed images. By employing multi-scale convolutional kernels to extract both local and global information, the generated structures not only exhibit geometrically realistic morphology, but also demonstrate favorable percolation and mechanical response characteristics^[13].

Despite significant advances in image-based 3D reconstruction methods, several limitations persist in

the existing literature. Firstly, while many statistical reconstruction approaches achieve satisfactory matches for low-order statistical descriptors, they often struggle to accurately reproduce realistic geometric morphology and topological characteristics across multiple scales. Traditional GAN methods frequently encounter issues such as mode collapse and gradient saturation when processing complex porous structures (*e.g.*, cement-based materials), thereby limiting effective generator training. Furthermore, current research rarely incorporates physical constraints (*e.g.*, porosity consistency) during the training process, resulting in deviations between the generated structures and target structures in terms of overall properties. Additionally, most network architectures remain relatively shallow, failing to effectively extract and represent hierarchical pore information, or they incur excessive computational costs that hinder their applicability to large-scale 3D data generation tasks.

To address the aforementioned challenges, a 3D high-fidelity reconstruction method based on Deep Convolutional Generative Adversarial Networks (DCGAN) is proposed in this paper, incorporating an autoencoder module within the generator to enhance multi-scale feature representation. The model introduces a porosity constraint term in the adversarial learning framework and integrates Wasserstein Generative Adversarial Networks with Gradient Penalty (WGAN-GP), significantly improving training stability and convergence performance. Trained on CT images of new silicate-aluminate cement paste at different curing ages, the model demonstrates outstanding performance in both geometric morphology and statistical feature consistency of the reconstructed results. Compared with traditional MJQA methods, the proposed approach shows substantial advantages in reconstruction accuracy and computational efficiency, providing an effective and reliable technical solution for modeling and simulating pore structure evolution in cement-based materials.

2 Experimental

The samples were prepared using the new

silicate-aluminate (limestone and calcined clay cement) system with 55% (mass fraction) Portland cement, 30% calcined clay, 15% limestone powder, and a water-to-binder ratio of 0.42. The cement paste samples were cast into cylindrical molds with a diameter of 1 cm and a length of 10 cm, demolded after 1 d, and then the samples were cut and polished into cylinders with a diameter of 1 cm and a length of 2 cm after standard curing (20 °C, 95% relative humidity) for 3, 28, 90 d, and 180 d. The samples were immersed in anhydrous ethanol to prevent further hydration. Finally, CT scans were performed on samples from all four curing ages. Fig.1 shows 2D slices and 3D schematic diagrams reconstructed from CT images. The geometric morphology and distribution characteristics of the pores in the images exhibit obvious randomness and heterogeneity. Each sample was prepared by fracturing to a width of approximately 1 cm prior to scanning for high-resolution microstructural characterization by micro-CT. Although the top and bottom surfaces of the samples were not perfectly level, the maximum cross-sectional width in the X-ray direction was maintained at about 1 cm. The height of the sample had no effect on the quality of the X-ray CT images. The resolution of the scanned images was 12.8 μm .

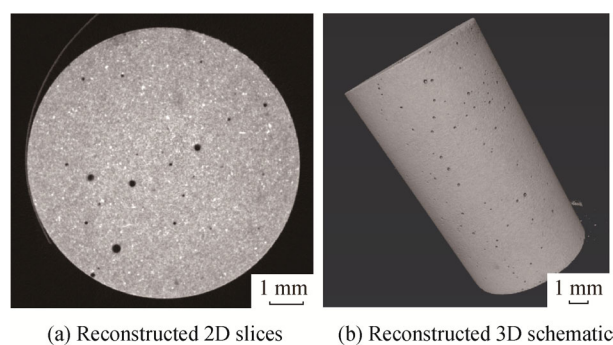


Fig. 1 2D slices and 3D schematic diagrams reconstructed from CT images

The CT data are composed of voxels, where the grayscale value of each voxel reflects the local matrix properties of the sample. Noise typically appears as random fluctuations in grayscale values, which can affect subsequent image processing and quantitative

analysis. To minimize such errors, a Gaussian filter is applied by convolving the image with a Gaussian kernel function, performing a weighted average on each voxel to smooth grayscale variations and eliminate random high-frequency noise. The process of threshold segmentation and the resulting 3D reconstructed images are shown in Fig. 2. Finally, the 3D images of the porous media were binarized to reduce the storage requirements of the training dataset. The binarized image is displayed in Fig. 3, where pores are represented by 0, while the unhydrated phase and hydrated product phase are represented by 1. 3D convolutional generative adversarial networks require a substantial volume of training samples, which necessitates extracting sub-volumes from the original 3D images. Excessively large image dimensions reduce the number of available samples and increase computational complexity during training. While overly small image sizes may fail to preserve the complete geometric characteristics of the porous medium, resulting in the generated images practically meaningless. In this study, a volume of 128 cubic micrometers was adopted as the size for individual training samples. The extracted training samples are shown in Fig. 4. At this scale, the images can effectively retain the geometric features of pores and their distribution characteristics.

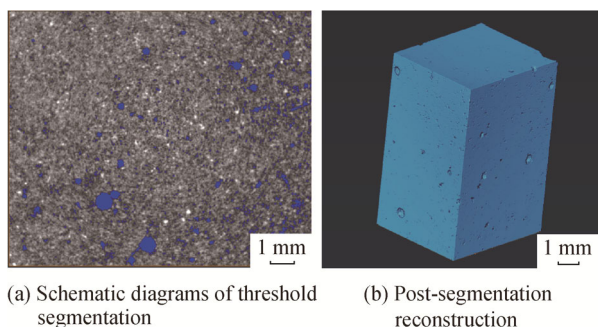


Fig. 2 Schematic diagrams of threshold segmentation and post-segmentation reconstruction

3 Theory

The 3D-to-3D reconstruction framework for cement-based materials was elaborated on, including the fundamental principles, loss functions, and network architecture.

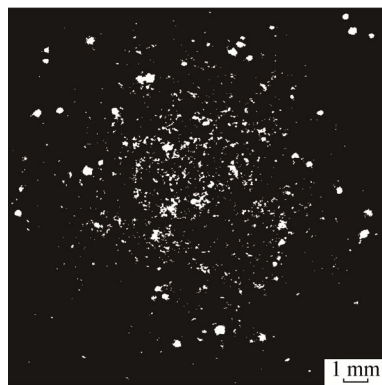


Fig. 3 Schematic diagram of binarized slices

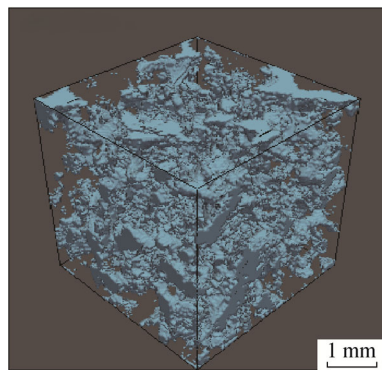


Fig. 4 Schematic diagram of representative volume element (RVE)

3.1 GAN

GAN is a generative neural architecture designed to produce synthetic data samples through an adversarial training process. This framework comprises two models trained simultaneously. One model is the generator G , which generates data based on the features of the original data, simulating the distribution of the training data. The other model is the discriminator D , which aims to distinguish between real samples and generated samples. These two models undergo adversarial training through their interaction, with the goal of making the features of the generated dataset resemble those of the original samples. Theoretically, balancing the generator and the discriminator is the most critical aspect of building a GAN model, which makes applying the correct loss function particularly important. The traditional loss function is as follows:

$$\min \max V(D, G) = \mathbb{E}_{z \sim p_z} [D(G(z))] - \mathbb{E}_{x \sim p_{\text{data}}(x)} [D(x)] + \lambda \mathbb{E}_{x \sim p_z} \left[\left(\|\nabla_x D(\hat{x})\|_2 - 1 \right)^2 \right] \quad (1)$$

Where $D(G(z))$ represents the critic's evaluation of the generated samples; $D(x)$ represents the critic's evaluation of the real samples; λ is a hyperparameter (regularization factor) that controls the importance of the gradient penalty term; $\nabla_x D(x)$ is the gradient of the critic's output with respect to the generated samples (used for enforcing the Lipschitz continuity).

The pore structure characteristics of cement-based materials are highly complex. The use of traditional GANs, which employ binary cross-entropy loss, is prone to gradient saturation and vanishing gradient problems, thereby hindering the update of the generator. This formulation also exhibits mode collapse behavior, preventing the generator from being effectively trained. To overcome these limitations and align with the characteristics of cement-based materials, the discriminator loss and the generator loss are expressed separately in this study. The discriminator loss function is defined as follows:

$$\text{Loss}_{\text{critic}} = -(\mathbb{E}[\text{critic}(\text{real})] - \mathbb{E}[\text{critic}(\text{fake})]) + \lambda_{\text{GP}} \cdot \text{Gradient Penalty} \quad (2)$$

Where $\mathbb{E}[\text{critic}(\text{real})]$ is the expected value of the discriminator's output for real samples; $\mathbb{E}[\text{critic}(\text{fake})]$ is the expected value of the discriminator's output for generated samples; λ_{GP} is the coefficient for the gradient penalty. The Gradient Penalty is the gradient penalty term, which aims to ensure that the discriminator's output is smooth, thus preventing mode collapse.

The generator loss function is as follows:

$$\text{Loss}_{\text{gen}} = -\mathbb{E}[\text{critic}(\text{fake})] + \lambda_{\text{porosity}} \cdot |\text{Porosity}(\text{fake}) - \text{Target Porosity}| \quad (3)$$

Where Porosity (fake) is the porosity of the generated samples; Target Porosity represents the actual porosity at different ages derived from CT data and calculated using Avizo; $\lambda_{\text{porosity}}$ is the weight for the porosity loss (experimentally tuned to minimize the discrepancy between the porosity of the generated structure and the target porosity).

3.2 Frame of model

Based on the above principles, a DCGAN architecture was constructed in this study, as shown in Fig. 5. The model couples a 3D generative adversarial

network with an autoencoder module. The encoder is used to extract multi-scale features of the pore structure, and the decoder is responsible for the reconstruction process, thereby enhancing the model's capability to represent complex structural features. The autoencoder strengthens multi-scale feature learning primarily by using the encoder to extract features at different scales from images or data. This process effectively captures multi-level structural information from the original images, ranging from local to global details^[14]. Particularly for materials with complex pore structures, such as cement paste, traditional single-scale feature learning often fails to adequately capture all the intricate details. In contrast, the autoencoder achieves a more comprehensive understanding of the pore structure through hierarchical abstract learning. Compared to traditional parallel multi-scale generative structures, the autoencoder achieves implicit multi-scale feature extraction through hierarchical latent variable learning, thereby avoiding coordination issues between different scale outputs in parallel structures. In this way, the autoencoder-coupled DCGAN model naturally integrates local details and global topological information within a single generation path, which enhances training stability and ensures consistency in reconstruction outcomes. In addition, to improve training stability and mitigate issues such as gradient vanishing, a gradient penalty term is introduced into the network, establishing a WGAN-GP framework based on the Wasserstein distance. This setup helps constrain the Lipschitz continuity of the discriminator, which alleviates oscillations during adversarial training and improves both the reliability of model convergence and the quality of the generated results. The penalty ensures Lipschitz continuity by penalizing gradients that deviate from unit norm, which are computed on interpolated samples between real and generated data. The encoder consists of three layers of 3D convolution, each followed by a ReLU activation function. Each convolution operation halves the resolution of the input data while increasing the number of feature channels. The output is a high-dimensional feature representation with a size of

$B \times 16 \times 16 \times 16 \times 16$, where B denotes the batch size. The decoder employs three layers of 3D transpose convolutions to progressively restore the spatial resolution of the input. The final layer employs a sigmoid activation function to normalize the data range $[0, 1]$, resulting in an output of size $B \times 1 \times 128 \times 128 \times 128$. The generator structure is similar to the decoder, as shown in Fig. 6. It also employs 3D transposed convolutions, but with GELU activation functions in the intermediate layers to produce smoother outputs. The generator ultimately produces a new 3D data output of dimensions $B \times 1 \times 128 \times 128 \times 128$. The discriminator consists of four layers of 3D convolution, as illustrated in Fig. 7. Each layer is followed by Instance Normalization and a Leaky ReLU activation function. The output is a small-sized

tensor of dimensions $B \times 1 \times 8 \times 8 \times 8$, which is used to determine whether the generated data is real or fake.

Although existing multi-GAN architectures are capable of extracting multi-level structural features through multi-scale generators, they often fail to provide effective control over porosity and global topology when reconstructing complex pore systems^[15]. To overcome these limitations, this paper introduces the WGAN-GP framework coupled with a porosity constraint. The proposed method ensures that the generated pore structures not only exhibit visual fidelity to real samples but also accurately conform to the target porosity, thereby significantly enhancing reconstruction accuracy. Furthermore, the generator effectively captures both local pore details and global structural characteristics across different scales by

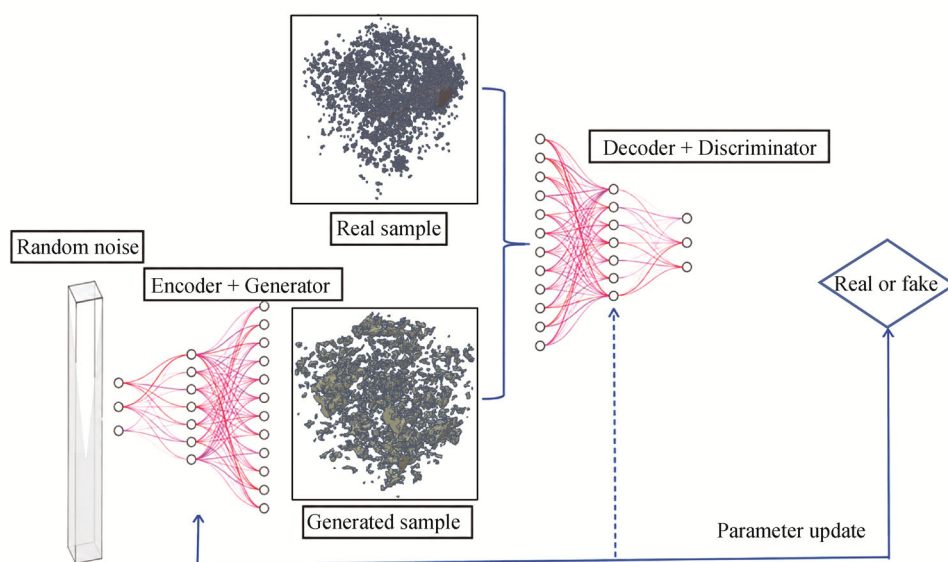


Fig. 5 Framework of the 3D DCGAN

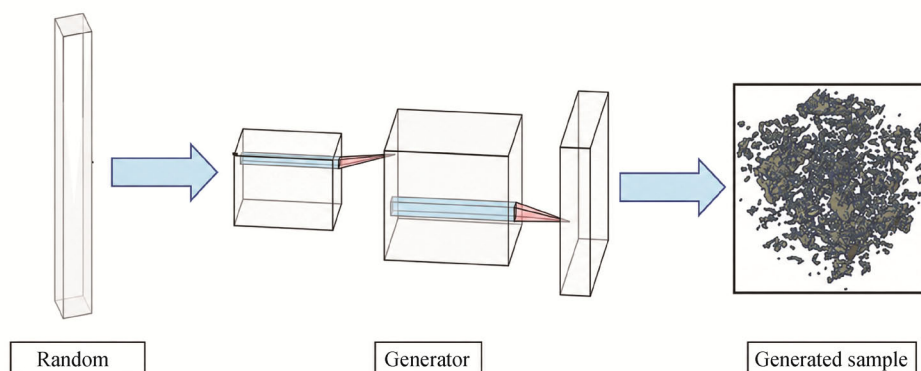


Fig. 6 Generator architecture of the DCGAN

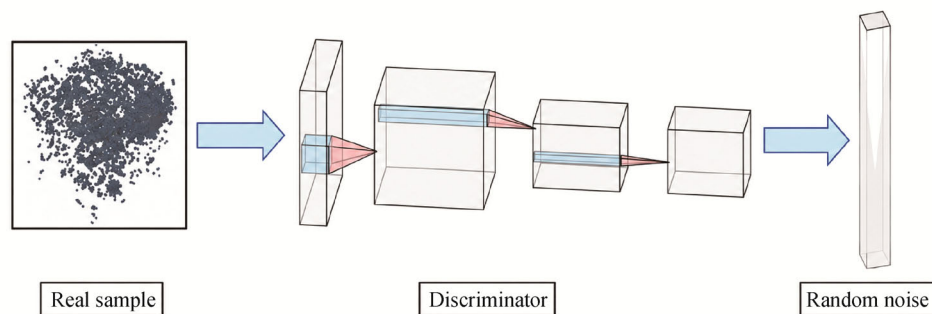


Fig. 7 Discriminator architecture of the DCGAN

incorporating a multi-scale feature extraction module based on an autoencoder, which overcomes the common shortcoming of conventional multi-GANs in detailed reconstruction. The adoption of WGAN-GP also enhances training stability and mitigates mode collapse, leading to improved training efficiency.

3.3 Training process

Based on the neural network framework described in the previous section, the 3D reconstruction of cement-based materials can be performed. The network construction and training in this study were implemented using the PyTorch deep learning framework. The training process is illustrated in Fig. 8, and the specific steps are as follows:

1) First, the hardened cement pastes need to be preprocessed. The method has been described in detail

in Section 1. This preprocessing supports a high-quality training process and improves the generalization capability and generation performance of the model.

2) The 3D DCGAN is constructed with specified convolution kernel size (k), stride (S), and padding (p). Both the discriminator (D) and generator (G) use the Adam optimizer to update network parameters, with settings such as learning rate configured accordingly.

3) During the initialization phase, the G parameters are first fixed. Fake samples are generated by inputting random noise, and both real and fake samples are fed into the D to assess authenticity and compute its loss function. Backpropagation is then used to update the parameters of the D , thereby enhancing its discriminative capability.

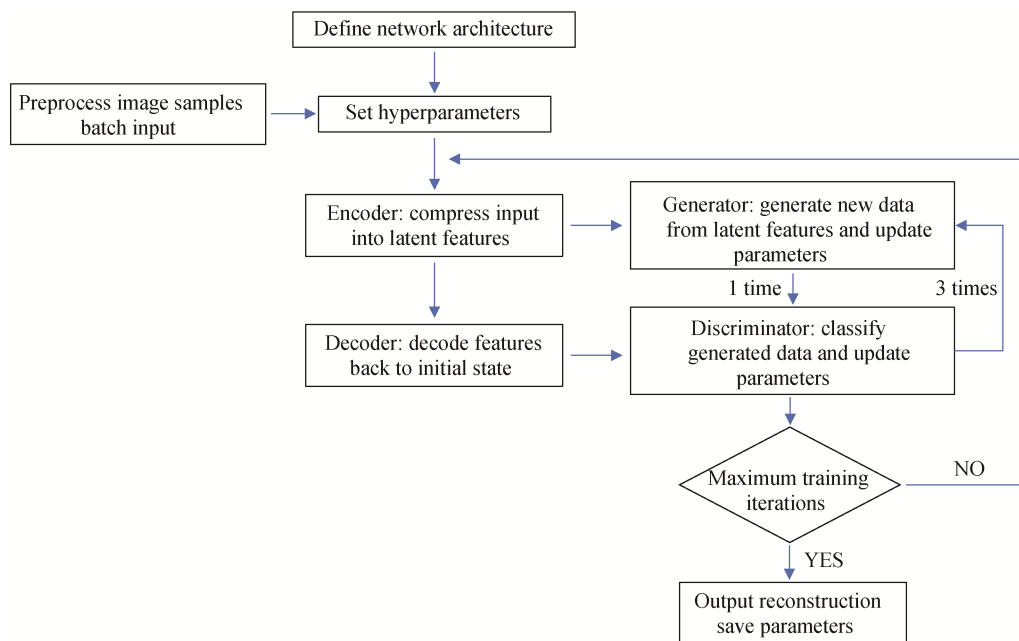


Fig. 8 Flowchart of neural network training

4) After training D for N_d iterations, its parameters are fixed. G produces batches of fake samples, which are then input into D for discrimination. The loss function is calculated, and backpropagation is performed to update the network parameters of G.

5) Steps 3) and step 4) are repeated until the maximum number of training iterations is reached, and the network parameters of G are saved. The trained G can rapidly produce reconstructed structures that follow the same distribution as the sample images.

4 Pore microstructure reconstruction analysis

4.1 Validation methodology and evaluation metrics

4.1.1 Minkowski functionals The Minkowski Functionals, proposed by the German mathematician Hermann Minkowski, are a class of important geometric measurement tools widely used to analyze the geometric morphology and topological characteristics of spatial structures^[16]. As a set of functions, the Minkowski functionals can be used to quantitatively characterize key geometric properties of objects in space, such as shape features, boundary attributes, and connectivity. In an n -dimensional space, there exist $n+1$ Minkowski measures. Thus, in a 3D image, there are four typical Minkowski functional metrics: volume (V), surface area (S), mean integral curvature (or mean width, M), and Euler characteristic (X)^[17]. Among these, the Euler characteristic is often referred to as the integral sum of Gaussian curvature and serves as an important topological parameter reflecting structural connectivity and the number of pores. The calculation expressions for the aforementioned Minkowski Functionals are as follows:

$$V=V(y) \quad (4)$$

$$S=\int_{\partial y} ds \quad (5)$$

$$M=\int_{\partial y} \frac{1}{2} \left[\frac{1}{r_1(s)} + \frac{1}{r_2(s)} \right] ds \quad (6)$$

$$X=\int_{\partial y} \frac{1}{r_1(s)r_2(s)} ds \quad (7)$$

Where $r_1(s)$ and $r_2(s)$ represent the maximum and minimum principal curvatures at a given surface point

s , respectively, reflecting the degree of local geometric variation of the surface.

4.1.2 Multiscale spatial statistical validation To comprehensively evaluate the accuracy of the reconstruction method, in addition to visual comparison and geometric metrics based on Minkowski functionals, this study further introduces multiple statistical functions to quantitatively analyze the generated and real volumes. In this section, four spatial statistical functions are employed: the two-point correlation function, lineal-path function, two-point cluster function, and two-point surface correlation function^[18–21]. These functions reveal the consistency and representativeness of structural distributions across different scales and perspectives. The mathematical definitions and physical significance of these correlation functions are illustrated in Fig. 9.

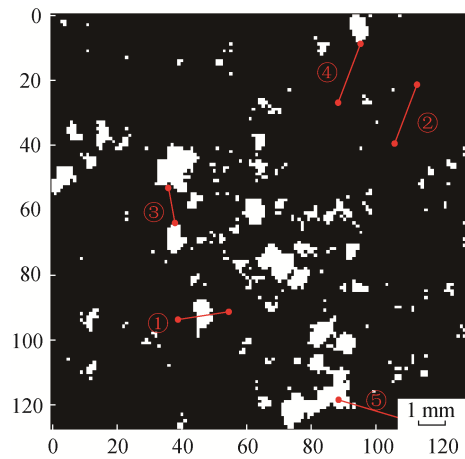


Fig. 9 Definitions of correlation functions: ① Two-point correlation function; ② Lineal-path function; ③ and ④ Surface correlation functions; ⑤ Two-point cluster function

1) Two-point correlation function.

The two-point correlation function $S_2(r)$ describes the probability that two points, separated by a distance r , are both located in the same phase (e.g., pore or matrix phase). It captures the spatial structural characteristics of pore and matrix distributions in porous media and is sensitive to both long-range and short-range correlations in the image. Due to its simple computation, it is widely used to characterize the statistical properties of porous media.

$$S_2(r) = P(x_1 \in \text{same phase as } x_2), \|x_1 - x_2\| = r \quad (8)$$

Where x_1 and x_2 represent two points in the image, and r is the distance between them.

2) Lineal-path function.

The lineal-path function $L(r)$ represents the probability that a line segment of length r in a given direction remains entirely within the same phase (e.g., pore phase). This function quantifies the connectivity and transport properties of pores in porous media and is particularly effective in evaluating whether the pore structure of generated images is interconnected and has a direct correlation with permeability and pore connectivity.

$$L(r) = P(\text{path of length } r \text{ in the same phase}) \quad (9)$$

3) Two-point cluster function.

The two-point cluster function $C_2(r)$, an extension of the two-point correlation function, represents the conditional probability that two points separated by a distance r belong to the same cluster within a given phase. It provides a quantitative description of the clustering characteristics of the pore phase, exhibits strong sensitivity to the short- and medium-range clustering behavior in complex porous structures, and effectively captures local heterogeneities in generated images.

$$C_2(r) = \frac{P(x_1, x_2 \in \text{same phase})}{P(x_1 \in \text{phase}) \cdot P(x_2 \in \text{phase})} \quad (10)$$

Where $P(x_1, x_2 \in \text{same phase})$ is the probability that both points belong to the same phase; $P(x_1 \in \text{phase})$. $P(x_2 \in \text{phase})$ represents the normalized probability under independent distribution.

4) Surface correlation functions.

The surface correlation functions describe the spatial correlation between surfaces and the pore or matrix phase, providing a quantitative measure of interface distribution and the interactions between adjacent phases. It reveals the uniformity and complexity of interface distributions in the generated images and is of great significance for evaluating pore shape, surface complexity, and interfacial characteristics.

The surface-surface correlation function $F_{ss}(r)$: the probability that two points separated by a distance r both lie on the phase interface.

$$F_{ss}(r) = P(x_1, x_2 \in \text{interface}), \|x_1 - x_2\| = r \quad (11)$$

The surface-phase correlation function $F_{sv}(r)$: the probability that, at a given distance r , one point lies on the interface while the other point is located within a specified phase.

$$F_{sv}(r) = P(x_1 \in \text{interface}, x_2 \in \text{specified phase}), \|x_1 - x_2\| = r \quad (12)$$

4.2 Reconstruction analysis

4.2.1 Reconstruction accuracy assessment based on Minkowski functionals First, reconstructions of the new silicate-aluminate paste were performed at different curing ages. As shown in Fig. 10, the apparent pore characteristics before and after reconstruction are highly similar, effectively reproducing the pore shapes and random distribution patterns. However, to validate the accuracy of the reconstruction beyond visual comparison, quantitative evaluation was conducted using the Minkowski functionals. Each 2D image was reconstructed three times to ensure the reliability of the results, and the average value of each correlation function was calculated as the final result.

Fig. 11 displays scatter plots based on these four metrics. The black scatter points represent the real data, while the red scatter points represent the generated data. The divergence between the two is highly consistent. This indicates that during the training process of the GAN, the addition of a discriminator for geometric parameters effectively constrains the geometric features of the generated images, confining their Minkowski parameters to a relatively accurate range. The comparison of porosity between the generated and real structures (Fig. 11a) validates the model's accuracy in satisfying the fundamental physical constraint. The relationship between specific surface area and porosity (Fig. 11b) reveals the model's capability to replicate geometric morphological complexity. The scatter plot of mean width versus porosity (Fig. 11c) is used to evaluate the fidelity of the model in restoring the multi-scale pore size distribution. The relationship between the Euler characteristic and porosity (Fig. 11d) provides a

rigorous examination of the topological connectivity as a high-order feature. The overall consistency in their complex distributions confirms that the generated

structures exhibit statistical similarity in essential topological attributes, such as pore-network connectivity and the number of isolated voids.

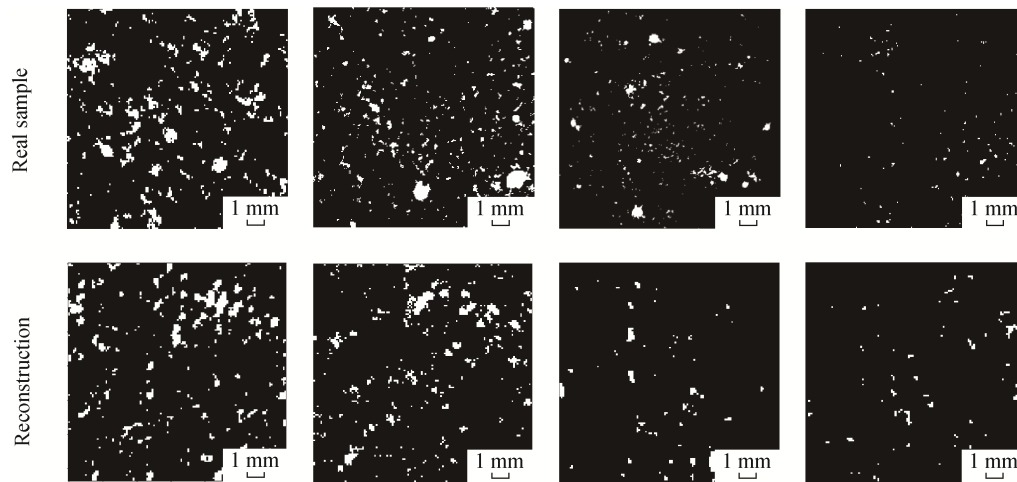


Fig. 10 Comparison of 2D slice results before and after reconstruction

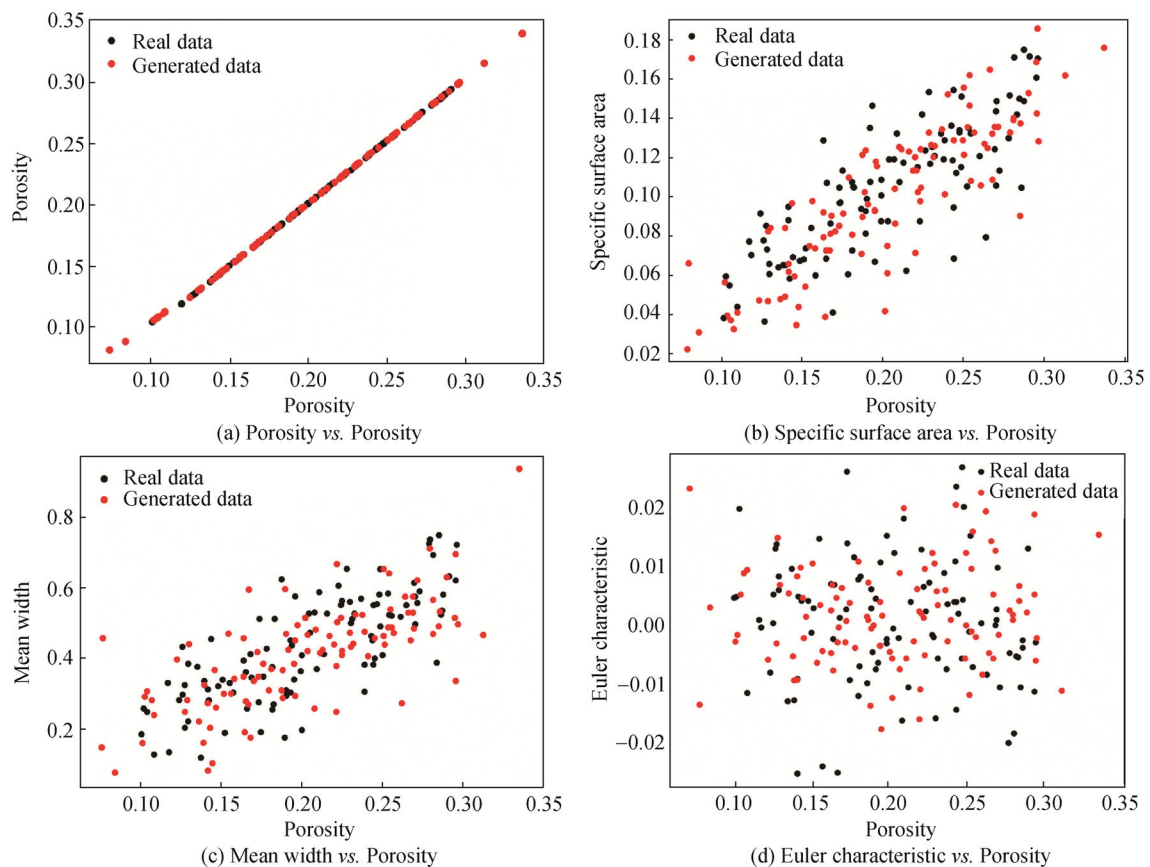


Fig. 11 Scatter plot of Minkowski parameters for 3D porous images

4.2.2 Reconstruction accuracy assessment based on statistical descriptors To further validate the reconstruction performance of the neural network, verification was conducted based on statistical

descriptors. The results are shown in Fig. 12. It can be observed that the statistical functions of the reconstructed results align well with those of the original structure, indicating that this reconstruction

method ensures statistical similarity.

4.3 Reconstruction efficiency

In addition, the reconstruction efficiency of the proposed method is further discussed. As shown in Fig. 13, the computation times of two reconstruction methods are presented for two different cases, with all hyperparameters kept constant. The purpose is to evaluate whether the coupled autoencoder in the network architecture improves training efficiency. As observed in Fig. 13, for the reconstruction process of a voxel size of $128 \times 128 \times 128$ under the same number of iteration cycles, the iterative efficiency is improved by approximately 150%. This demonstrates the significant advantage of the proposed method in reconstruction efficiency. This is primarily because the method is fundamentally based on a neural network composed of four subnetworks. Once training is completed, the reconstruction process only

involves operations on parameter matrices. In contrast, traditional methods consist only of a generator and a discriminator, and the convergence is much slower under unequal backpropagation. This mechanism inherently limits the ability to achieve high reconstruction efficiency. Although traditional GANs achieve considerable reconstruction accuracy, their training process is often protracted and computationally inefficient. The absence of effective structural constraints in conventional methods introduces significant oscillations and instability during training, resulting in slow convergence. By contrast, the proposed approach—integrating WGAN-GP and porosity constraints—employs a more stable adversarial training framework augmented with physical regularizations, markedly improving convergence speed and generation efficiency.

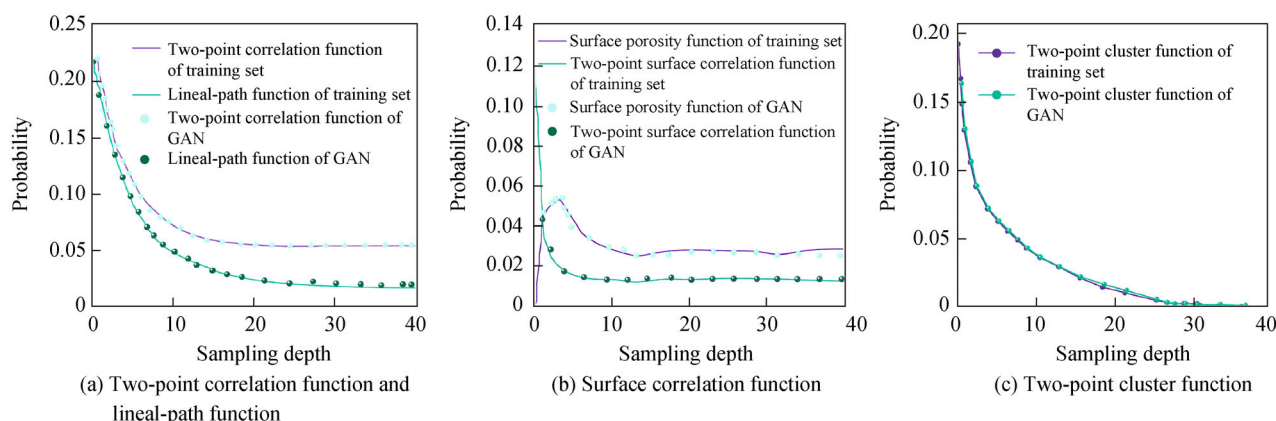


Fig. 12 Statistical descriptor analysis of 2D paste microstructure images

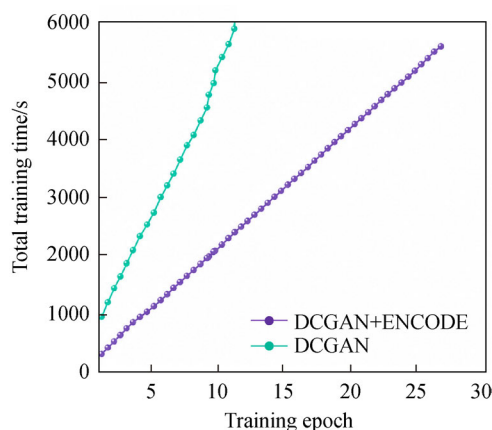


Fig. 13 Comparison of time consumption between two methods

5 Conclusions

This study constructs an efficient 3D GAN model based on CT images of cement paste, achieving high-precision 3D reconstruction of pore structures at different curing ages. The main conclusions are as follows:

1) A 3D pore structure reconstruction method was proposed. Using measured pore images at different curing ages as training samples, a DCGAN was trained to achieve 3D image generation and modeling of the pore evolution process in cement-based materials.

2) A coupled GAN–autoencoder architecture was constructed to strengthen multi-scale feature learning and denoising, thereby improving reconstruction fidelity. Meanwhile, a porosity constraint was incorporated into adversarial learning to ensure global consistency of the generated pore structure with real samples.

3) By introducing a gradient penalty term, the training stability and convergence efficiency were improved. Combined with structural optimizations such as the ReLU and GELU activation design in the generator and Instance Normalization in the discriminator, the generation quality and generalization capability were further enhanced.

4) The accuracy and reliability of the model in terms of morphological structure and porosity control were validated through quantitative indicators such as Minkowski functionals and statistical descriptors, along with visual comparisons. Moreover, the computational efficiency was significantly improved (by approximately 150%).

The 3D deep generative model constructed in this study not only demonstrates good stability and robustness during training but also achieves high-quality reconstruction of pore structures in cement-based materials while maintaining structural diversity and realism.

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Three-Dimensional Reconstruction of Pore Structure in Hardened Paste *via* Generative Adversarial Networks

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Extended Abstract

Introduction In recent years, the continuous development of 3D reconstruction methods for porous media has promoted the integrated evolution of image modeling, performance prediction, and multiscale microstructure analysis. Although traditional reconstruction approaches achieve satisfactory matches for low-order statistical descriptors, they often struggle to accurately reproduce realistic geometric morphology and topological characteristics across multiple scales. Meanwhile, traditional generative adversarial network (GAN) methods exhibit remarkable advantages in handling complex porous structures (*e.g.*, cement-based materials), yet are prone to issues such as mode collapse and gradient saturation. To address the aforementioned challenges, a high-fidelity 3D reconstruction method based on deep convolutional generative adversarial networks (DCGANs) is proposed in this paper, incorporating an autoencoder module within the generator to enhance multiscale feature representation. The model introduces a porosity constraint term in the adversarial learning framework and integrates Wasserstein generative adversarial networks with gradient penalty (WGAN-GP), significantly improving training stability and convergence performance. Trained on CT images of new silicoaluminate cement paste at different curing ages, the model demonstrates good performance in both geometric morphology and statistical feature consistency of the reconstructed results.

Methods The samples were prepared using the new silicoaluminate (limestone and calcined clay cement) system with 55% (mass fraction) Portland cement, 30% calcined clay, 15% limestone powder, and a water-to-binder ratio of 0.42. High-resolution micro-CT images were obtained at curing ages of 3, 28, 90 d, and 180 d. The images were preprocessed using Gaussian filtering and threshold segmentation to obtain binarized pore structures. A DCGAN architecture was developed by integrating 3D generative adversarial networks (GANs) with an autoencoder module. The framework incorporated gradient penalty to establish a WGAN-GP based on the Wasserstein distance, thereby constraining the Lipschitz continuity of the discriminator. A porosity constraint term was introduced into the adversarial learning framework to ensure global statistical consistency of the reconstructed microstructures. The reconstructed 3D volumes were validated against experimental microstructures using Minkowski functionals (porosity, surface area, Euler characteristic) and spatial correlation descriptors including the two-point correlation function (S_2), lineal-path function, two-point cluster function, and surface correlation function.

Results and discussion The results demonstrate that the proposed model effectively reconstructs pore morphology and distribution characteristics across different curing ages, with the porosity of reconstructed volumes showing good consistency with measured samples. The introduction of a gradient penalty term in the loss function enhanced the training stability and convergence efficiency of the model. By incorporating porosity as a regularization term in the adversarial learning framework, the model was effectively guided to learn the porosity evolution trends across different curing ages, thereby improving the consistency between generated structures and experimental data. The generator employed a combined ReLU and GELU activation mechanism, which contributed to stable generator training. The integration of Instance Normalization in the discriminator further improved the quality of generated results and the generalization capability of the model. Comparative analyses based on Minkowski functionals and statistical descriptors revealed that the generated structures exhibit high agreement with the original CT images in terms of geometric morphology, connectivity, and spatial correlation. Compared to conventional reconstruction methods, the proposed approach improves computational efficiency by approximately 150% while maintaining structural fidelity.

Conclusions This study constructed an efficient 3D generative adversarial network (GAN) model based on CT images of cement paste, achieving high-precision 3D reconstruction of pore structures at different curing ages. The proposed model demonstrates good stability and robustness during training and achieves high-quality reconstruction of pore structures in cement-based materials while effectively preserving structural diversity and morphological realism.

Keywords hardened paste; neural network; CT images; pore structure; three-dimensional reconstruction