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Automated image segmentation of 3D printed fibrous composite micro-structures using a neural network

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ABSTRACT

A new, automated image segmentation method is presented that effectively identifies the micro-structural objects (fibre, air void, matrix) of 3D printed fibre-reinforced materials using a deep convolutional neural network. The method creates training data from a physical specimen composed of a single, straight fibre embedded in a cementitious matrix with air voids. The specific micro-structure of this strain-hardening cementitious composite (SHCC) is obtained from X-ray micro-computed tomography scanning, after which the 3D ground truth mask of the sample is constructed by connecting each voxel of a scanned image to the corresponding micro-structural object. The neural network is trained to identify fibres oriented in arbitrary directions through the application of a data augmentation procedure, which eliminates the time-consuming task of a human expert to manually annotate these data. The predictive capability of the methodology is demonstrated via the analysis of a practical SHCC developed for 3D concrete printing, showing that the automated segmentation method is well capable of adequately identifying complex micro-structures with arbitrarily distributed and oriented fibres. Although the focus of the current study is on SHCC materials, the proposed methodology can also be applied to other fibre-reinforced materials, such as fibre-reinforced plastics. The micro-structures identified by the image segmentation method may serve as input for dedicated finite element models that allow for computing their mechanical behaviour as a function of the micro-structural composition.

1. Introduction

Fibre-reinforced materials are used in a wide range of engineering applications. Within the field of additive manufacturing, various fibrous composites have been recently developed and improved to obtain an optimal strength and deformation behaviour during the structural processing and application stages. A typical example concerns the strain-hardening cementitious composites (SHCC) used for extrusion-based 3D concrete printing applications [1–5], see Fig. 1. The assessment of the mechanical performance of such a material requires detailed information of the spatial distribution and orientation of fibres. This can be accomplished by X-ray micro-computed tomography (μCT) [6], which uses X-rays to create cross-sectional images of the material sample. The 3D scan constructed from these images, or ‘slices’, is composed of a group of voxels, with the local material density of a voxel being indicated by a grey scale value. The size of the scanned specimen volume commonly is limited, and tuned to the smallest micro-scale object of interest (e.g., fibre, air void, matrix material). The identification of the locations and boundaries of the objects is accomplished by image segmentation; for air voids [7] and steel fibre reinforcement in concrete [8], this technique is relatively straightforward to apply, as the difference in density then is sufficiently large for using threshold grey scale values to unequivocally identify these micro-structural objects from a 3D scan. Conversely, for an SHCC reinforced by polyvinyl alcohol (PVA) fibres, the result of image segmentation may become inaccurate, since the grey scale values of the fibre voxels considerably overlap with those of the matrix and air void voxels [3], see Fig. 2. Consequently, simple segmentation techniques, such as histogram thresholding [9] and feature extraction [10], do not work adequately under these circumstances. Nevertheless, given the fact that there is sufficient image context around each voxel, by carefully analysing the 3D morphology of the fibres, a domain expert would still be able to determine if a particular voxel belongs to a fibre or not. Moreover, the task of image segmentation by a human expert can be efficiently automated by applying machine learning techniques.

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in the form of a convolutional neural network, as demonstrated by successful applications in the fields of medicine [11], radiology [12], and cyber security [13].

The potential of a deep convolutional neural network (DCNN) for the segmentation of PVA fibres in SHCC has been recently demonstrated in [14]. In this contribution, the machine learning problem is considered to be ‘supervised learning’, whereby a human expert manually generates sufficient examples of segmented images that in turn are used to train the neural network for image segmentation. Note, however, that the manual annotation of micro-structural objects in 3D printed SHCC materials is cumbersome, because fibres may be oriented in arbitrary directions and practically never are located in a single plane [3], see also Fig. 2. Consequently, it is necessary to consider each voxel from multiple angles for determining to which specific class the micro-structural objects of interest belong. In order to practically solve this issue, in the present paper a new methodology is proposed, in which the image segmentation of fibre-reinforced materials is performed with automated annotations of physical sample data. For this purpose, a training sample is prepared of a single yarn of fibre embedded in a cementitious matrix, whereby the location and main orientation of the fibre are defined a priori and established as ground truth. The air void and matrix are effectively segmented by means of threshold filtering, resulting in a complete 3D ground truth mask of the scanned specimen. The ground truth data of the single-fibre specimen is next subjected to a data augmentation procedure, in order to allow for the automated identification of fibres oriented under arbitrary directions. Accordingly, the need of a human expert for manually annotating these data becomes redundant. The augmented dataset is used to train a 3D convolutional neural network with U-Net architecture to segment randomly distributed and oriented fibres from the cementitious matrix and air voids. The applicability of the methodology is demonstrated by network predictions of the complex fibrous micro-structure of an SHCC material developed for 3D concrete printing. Although the focus of the current study is on SHCC materials, the proposed methodology can also be applied to other fibre-reinforced materials, such as fibre-reinforced plastics [15].

The micro-structures identified by the present image segmentation method may serve as input for dedicated finite element models in which the local interactions between fibres and matrix material are simulated in detail [16,17], and from which the effective mechanical properties (elastic modulus, yield strength, fracture strength, toughness) in the fresh and hardened states can be determined as a function of the micro-structural composition by applying advanced homogenization techniques [18–20]. The effective mechanical properties of fresh SHCC micro-structures are needed for designing against failure (elastic buckling, plastic collapse) and undesirable deformations during a 3D printing process, and for the optimization of manufacturing parameters, such as the printing speed and the usage of printing material [21–25].

This paper is organized as follows. Section 2 introduces the automated image segmentation method of fibre-reinforced materials by presenting a detailed overview of the individual steps of the training and application phases of the neural network. Section 3 demonstrates the applicability of the method using three types of SHCC developed for 3D concrete printing. An overview is provided of the material compositions, specimen preparation, and scanning and masking procedures, after which micro-structural segmentation results computed by the neural network are compared for three different training datasets characterized by a decreasing directional bias of the fibres. Subsequently, the predictive capability of the method is demonstrated via the analysis of a practical SHCC material characterized by a micro-structure with a large number of arbitrarily distributed and oriented fibres. Section 4 summarizes the main conclusions of the study, both regarding the image segmentation methodology in general and the SHCC material in particular.

2. Image segmentation method

The proposed image segmentation method is based on the assumption that the fibres in the matrix appear as (virtually) straight at a sufficiently fine, local scale. Accordingly, an accurate dataset can be created through the 3D scanning of a basic specimen composed of a single, prestressed (and therefore straight) yarn of fibre surrounded by a cementitious matrix with air voids, and dividing this scan into smaller windows of which the dimensions correspond to those at which fibres in real fibre-reinforced materials appear as straight. Nevertheless, these training data, which are based on one specific (vertical) fibre orientation, refer to only a small part of the overall data collection that includes all possible fibre orientations. In order to generalize the DCNN algorithm, it is important that representative training data from a data collection, or ‘data manifold’, with all possible fibre orientations is used. This can be achieved by a data augmentation procedure, whereby the windows of the obtained scan are rotated along three perpendicular coordinate axes under arbitrary angles, after which the neural network can be trained for the segmentation of samples with arbitrarily oriented fibres. The methodology to efficiently train a DCNN to segment randomly distributed and oriented fibres from a matrix with air voids consists of 5 separate steps, as illustrated in the flowchart in Fig. 3. Each of these steps is explained in more detail in the subsections below.

2.1. Physical training specimen

The first step of the proposed methodology concerns the preparation of the specimen needed for the training of the neural network. For this purpose, the basic, single-fibre SHCC specimen presented in Fig. 4(left) is used, which contains a yarn of straight fibre embedded in a cementitious matrix material with air voids. The specimen has a cylindrical shape, in order to avoid scanning artefacts due to size variations along the outer boundary of the specimen. The specimen is prepared inside a plastic cylinder by adding cementitious matrix material in a layered-wise fashion. Polystyrene foam is used to close the top and bottom sides of the plastic cylinder during curing, and to attach the fibre. The fibre is straightened under its self weight, after which the specimen is exposed to a curing period of minimally 14 days. More details of the specimen preparation procedure are provided in Section 3.2.
that is smaller than the actual cross-section of the fibre. Further, the resolution. This effect can be kept limited by applying a fibre mask whereby the degree of enlargement depends on the applied scanning fibre typically may appear somewhat larger than the actual width, \( \mu \) matrix material. Consequently, in the of the fibre and the adjacent air void, or the fibre and the adjacent which results in edge voxels showing greyscale values between these the fibre edge generally does not coincide with the edge of a voxel, thus maintaining clear object edges at these transitions.

2.2. Micro-computed tomography scanning

In the second step of the methodology, a digital 3D representation of a part of the specimen is constructed using \( \mu \)CT scanning, see Fig. 2(middle). The scanning volume of the sample is the product of the voxel size and the total number of voxels, of which the latter has a fixed maximum. For obtaining a representative scan of the micro-structure at an adequate resolution, a sufficiently large scanning volume and a sufficiently small voxel size need to be selected, as specified in Section 3.2. A \( 3 \times 3 \times 3 \) 3D median filter is used for reducing the noise in the scanning volume without enlarging the transition zones between the different micro-scale objects (i.e., fibre, air void and matrix), thus maintaining clear object edges at these transitions.

2.3. Pre-processing

In the third step, the pre-processing of the obtained 3D volume of the training specimen is performed, after which it can be used as input for the neural network. The pre-processing procedure creates a labelled specimen volume, named the ‘ground truth mask’, by allocating for each voxel the associated label of ‘matrix’, ‘air void’ or ‘fibre’. The procedure starts with constructing the mask for the fibre. The yarn of fibre is straight, due to a prestress generated in the yarn before applying the matrix material. The central voxel of the yarn is selected manually at every 100th slice, after which a linear interpolation procedure is used to efficiently determine the central voxels in each of the 99 intermediate slices, see Fig. 4(middle). Depending on the type of fibre used, it is possible that the diameter of the fibre is only a few times the voxel size. To complete the mask for the fibre, the voxels located within the actual fibre diameter have to be labelled as ‘fibre’. However, the fibre edge generally does not coincide with the edge of a voxel, which results in edge voxels showing greyscale values between these of the fibre and the adjacent air void, or the fibre and the adjacent matrix material. Consequently, in the \( \mu \)CT scans the imprint of the fibre typically may appear somewhat larger than the actual width, whereby the degree of enlargement depends on the applied scanning resolution. This effect can be kept limited by applying a fibre mask that is smaller than the actual cross-section of the fibre. Further, the centreline of the fibre needs to be accurately determined, as it defines the centreline of the fibre mask. The complete mask of the micro-structure is finally obtained by the segmentation of air voids and matrix, which can be straightforwardly accomplished with threshold filtering. The top and bottom slices are removed from the mask if large scanning artefacts are visible in the scanned image, after which the procedure continues by cropping the original 3D volume to the same size as the mask. Subsequently, contrast stretching is applied, whereby the greyscale values are scaled over the range of values characterizing the scanned 3D volume. Finally, these integer values are rescaled to real numbers between 0 and 1, as required for calculations with the neural network. The ground truth mask resulting from the above procedure is illustrated in Fig. 4(right). The figure has been deduced from a three-dimensional representation, whereby the cementitious matrix has been made transparent. Hence, the fibre (indicated in red) and air voids (indicated in grey) are shown in the depth direction of the sample.

2.4. Data augmentation

The data obtained from the pre-processing step only contain part of a yarn of fibre in a very specific (vertical) direction, see Fig. 4(right). Preliminary trials showed that with these data the DCNN algorithm indeed works inadequately for material samples containing randomly oriented fibres, as it will only recognize fibres oriented in the same (vertical) direction as represented in the training dataset. This directional bias is elaborated in more detail in Section 3. In order to overcome this bias, in the fourth step of the methodology the training dataset is augmented artificially, such that it contains all possible fibre orientations in equal proportions. A simplified, 2D representation of this data augmentation approach is presented in Fig. 5. Accordingly, the 3D cropped ground truth mask shown in Fig. 4(right) is first divided into a batch of cubic \( a \times a \times a \) voxel windows, each of which is subsequently rotated over the full range of possible rotation angles along three orthogonal coordinate axes. After each rotation, the rotated cubic voxel window is cropped to an internal, straight cube of size \( b \times b \times b \), and added to the training dataset. Since the above procedure also rotates the 3D voxel structure, a trilinear interpolation scheme is applied to re-establish the original greyscale pattern. Other interpolation schemes are inadvisable, as they tend to change greyscale values by smoothening the contrast between the micro-scale objects (i.e., fibre,
Fig. 3. A flowchart indicating the individual steps during the training phase (left) and use-phase (right) of the neural network. The 5 individual steps of the training phase are explained in Sections 2.1 to 2.5, respectively, and the use-phase is explained in Section 2.6.

Furthermore, the size $a$ of the voxel window is determined by multiplying the required cube edge $b$ with a factor $\sqrt{3}$, i.e., $a = b\sqrt{3}$, which ensures that the window completely overlaps the internal cube under

air void, matrix). The edge length $b$ of the internal, straight cube needs to be selected such that fibre parts within, which are representative of the real, use-phase specimen, appear as (approximately) straight.
Fig. 4. Schematic overview for obtaining ground truth data for the neural network from a basic, single-fibre SHCC specimen. Left: Representation of the construction of the SHCC specimen, using a [1]: PVA yarn, [2]: closed-cell extruded polystyrene foam, [3]: cementitious matrix and [4]: plastic cylinder. Middle: Vertical μCT-slice of the specimen, with the rectangular mask constructed by interpolating the longitudinal fibre geometry from the locations of the central voxel of every 100th horizontal slice (indicated by a white horizontal line). Right: Ground truth mask for a selected part of the μCT-scanned specimen, distinguishing the PVA fibre (red line), the air voids (grey region) and the cementitious matrix (transparent region). The transparent representation of the matrix provides an in-depth front view of the 3D mask, as a result of which the air voids appear somewhat different than in the vertical slice of the μCT scan shown in the middle. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 5. A schematized 2D representation of the data augmentation procedure for a rotation angle of 45°. The area of the voxel window is \( a \times a \), and contains \( 8 \times 8 = 64 \) voxels (pixels) in this example. The reduced, internal area of the voxel window is \( b \times b \), with \( a = \sqrt{2} b \). In the 3D representation of this procedure, the factor \( \sqrt{2} \) relating the voxel window size \( a \) to the edge length \( b \) increases to \( \sqrt{3} \).

all possible rotations. Specifically, the factor of \( \sqrt{3} \) is determined by the most critical combination of an in-plane rotation of 45 degrees, followed by an out-of-plane rotation of 45 degrees. Observe that in Fig. 5 this factor is represented by \( \sqrt{2} \), in correspondence with a single (in-plane) rotation of 45 degrees in the schematized 2D representation.

2.5. Deep convolutional neural network

The fifth step of the methodology refers to the training of a convolutional neural network with a U-Net architecture [26]. The specific features of this U-Net architecture were chosen after a preliminary parameter variation study, in which the size and amount of convolutional layers (i.e., the main building blocks of the DCNN) were varied. The final architecture is illustrated in Fig. 6. The selected architecture follows from a workable balance between the number of trainable parameters and the convergence time experienced during training. Observe that the network has a width of 3 levels and a depth of 15 layers. The convolution size of each horizontal connection between the layers corresponds to \( 3 \times 3 \times 3 \) voxels, except for the output layer where a \( 1 \times 1 \times 1 \) convolution size is used. Constant padding is applied to retain the original image size during convolutions. For the vertical connections between levels a max pooling and deconvolution size of \( 2 \times 2 \times 2 \) voxels is used [27]. The filters at the first level of the DCNN have an effective range of \( 3 \times 3 \times 3 \) voxels, in correspondence with the convolution size of \( 3 \times 3 \times 3 \) voxels. At the second level, this effective range becomes \( 6 \times 6 \times 6 \) voxels after a \( 2 \times 2 \times 2 \) max pooling of the first level. At the third level, an effective range of \( 12 \times 12 \times 12 \) voxels is reached after another \( 2 \times 2 \times 2 \) max pooling. The skip connections shown in Fig. 6 connect the layers at the same level with each other, in order to avoid loss of information to a deeper level. Within the hidden layers of the network, rectified linear unit (ReLU) activation functions are used, which tend to speed up the convergence rate of the neural network calculation [28]. The hidden layers are initialized with He (or Kaiming) initialization that is based on the shape of the network [29], and accounts for the non-linearity of the ReLU activations. The output layer of the neural network has a softmax activation function in order to obtain for each voxel a prediction between 0 and 100% class probability for all three micro-scale objects (i.e., fibre, air void or matrix) [30], whereby the sum of the predicted percentages of the three objects equals 100%. The incremental-iterative update procedure required for an accurate training of the network is performed with the stochastic gradient-descent algorithm ‘Adam’, using a batch size of 64.
samples and a learning rate of 0.001 [31]. The learning rate scales the step size adopted in the update procedure, in order to minimize the overall categorical cross-entropy or 'loss' (which is further defined in Section 3.3). For avoiding overfitting of the network, at each level a regularization method called 'drop-out' is added to the second convolution layer [32]. The convolutional neural network is constructed using Python, thereby applying the Tensorflow [33] and Keras [34] packages. The dataset characterizing the ground truth of a micro-structure is used for calculating the absolute error in the prediction of the specific micro-scale object in each voxel, after which the filters are updated for each batch of the dataset using backpropagation. In the training phase, weighting factors are applied to compensate during backpropagation for the appearance frequency of each class, which avoids that the network strongly overpredicts the largest class (i.e., the cementitious matrix). The validation data, which have not been used for the training of the network, serve to check whether the accuracy of the network calculation for these data is similar as for the training data. If the accuracy during validation is smaller, it is concluded that the network has been trained insufficiently accurate (i.e., the result computed by the network does not generalize well), so that the training phase needs to be redone with a larger, more representative, amount of training data.

The training and validation phases of the neural network are divided into a certain number of epochs. An 'epoch' refers to a certain time instant in the incremental( iterative) time-stepping procedure applied during the training and validation of the neural network. An individual epoch is considered to be finished when the full training dataset or validation dataset has been sent through the network once. During training, each epoch consists of a fixed amount of iterations, whereby the selected value is based on the size of the training dataset. The amount of epochs needed for obtaining an accurate prediction of the ground truth mask is determined by the convergence rate of the neural network, which is selected based on the highest percentage prediction. From the class predictions on each patch, the overall segmentation of the 3D printed SHCC sample is reconstructed using the original patch locations. Steps applied during the training phase, see the overview in Fig. 3. The use-phase specimen is obtained by drilling a cylindrical sample from a hardened, 3D printed SHCC beam. The specimen is scanned by applying a similar scanning procedure as for the single-fibre specimen used for the training and validation of the network. However, the pre-processing step for the use-phase specimen is different from that of the training specimen. Initially, the image is cropped around the specimen, after which contrast stretching is applied whereby the greyscale values are scaled over the range of values characterizing the 3D volume of the specimen. Since the neural network has been trained with a specific window size of $b \times b \times b$ voxels, see Fig. 5, the 3D images are divided into patches of this window size. The original locations of the patches are stored for reconstructing the geometry of the micro-structure in the post-processing stage, after the neural network calculations are finished, in accordance with step 6 in the flowchart in Fig. 3. Similar to the training specimen, the greyscale integer values that represent the densities of the scanned 3D volumes are rescaled to real density values between 0 and 1, as needed for calculations with the neural network. For each voxel on a patch, the neural network determines a percentage prediction for the class probability of the three possible classes of micro-scale objects. The final class of micro-scale object of each voxel is selected based on the highest percentage prediction. From the class predictions on each patch, the overall segmentation of the 3D printed SHCC sample is reconstructed using the original patch locations.

3. Application to printable SHCC samples

3.1. Experimental program

The image segmentation method developed in Section 2 is applied to various SHCC samples. Accordingly, three physical training specimens with different material compositions were manually prepared, which are referred to as the 'X-mix', '1A-mix' and the '1B-mix', see Table 1. From the scan of the X-mix specimen, three datasets were created: one unidirectional dataset based on the original scan, in which only the vertical fibre orientation is considered, one orthodirectional dataset whereby the unidirectional training and validation data were augmented by applying an image rotation procedure that only uses right ($+90$ degrees, $-90$ degrees) and straight (180 degrees) rotation angles along the three orthogonal coordinate axes, and one omnidirectional dataset whereby the unidirectional data were augmented by applying...
an image rotation procedure based on arbitrary rotation angles, as described in Section 2.4. The comparison of the training and validation results of the network for these three datasets will demonstrate for the single-fibre specimen how the manifold of fibre orientation angles influences the accuracy and corresponding convergence rate of the network. In addition to the X-mix, from the scans of the 1A-mix and 1B-mix specimens omnidirectional datasets were created. The accuracy of the network prediction during training and validation is assessed for the three mixes, and for each mix the predicted segmentation of the micro-structure of the single-fibre specimen is compared to the corresponding ground truth mask. Finally, a use-phase specimen with randomly distributed PVA fibres oriented in arbitrary directions was 3D printed using the X-mix composition, and was subsequently analysed with the neural networks created from the omnidirectional training datasets of the X-, 1A- and 1B-mixes. The experimental procedure and results are discussed in the subsections below.

### 3.2. Specimen preparation, scanning and masking

From the three mix designs listed in Table 1, three corresponding, physical specimens were prepared. The composition of the X-mix was taken from [1], and the compositions of the 1A- and 1B-mixes were taken from [35]. The three mix designs were developed for 3D concrete printing applications and contained 2% (by volume) oil-coated PVA fibres (RECS15) with a length of 8 mm and a diameter of 40 μm. However, for the single-fibre specimens used for the training and validation of the neural network, the volumetric fibre percentage is much lower, between 0.02% and 0.04%. Fig. 7 shows the voxel density probability distribution for the three mixes, as determined from the ground truth mask of the single-fibre specimen after contrast stretching. Note that the voxel densities are scaled between 0 and 1. The voxel density probability distributions of the X- and 1B-mixes are in close agreement, while the voxel density probability distribution of the 1A-mix is significantly different. These resemblances and differences in the voxel density probability distributions of the three selected mixes allow for a systematic examination of the effect of the level of agreement in voxel density probability distribution on the accuracy of the image segmentation result. The normalized densities of the air voids, fibres and cementitious matrix roughly correspond to values in the ranges 0–0.3, 0.2–0.5 and 0.4–1.0, respectively.

The preparation of the training specimen (one per mix design) started by placing a yarn of fibre through a round piece of polystyrene foam, which was put inside a plastic cylinder with an inner diameter of 15 mm, as shown in Fig. 4(left). The polystyrene foam was used to close the bottom of the plastic cylinder. In order to prevent the movement of the yarn of fibre through the polystyrene foam, the end of the fibre was taped to the plastic cylinder. Subsequently, the matrix material was added around the fibre in 10 batches of approximately 1 ml, followed by compacting the specimen for 15 s on a shaking table. The fibre was then passed through another piece of polystyrene foam that closes the cylindrical plastic cylinder from the top. The yarn was straightened under its self weight, after which the specimen was exposed to a curing period of minimally 14 days. Table 2 presents the volumetric percentages of the matrix, fibre and air void phases in the hardened, single-fibre ground truth specimens prepared with the X-mix, 1A-mix and 1B-mix. Note that the fibre percentages of the three mixes show small differences; this results from the fact that the ground truth masks of the fibre for the three mixes were composed of the same number of voxels, but the total ground truth masks (which also includes the air voids and matrix) were characterized by slightly different numbers of voxels. It can be further seen that the X-mix contains the largest amount of air voids, followed by the 1B-mix and finally the 1A-mix.

Fig. 8 shows an SHCC specimen inside a Phoenix Nanotom μCT-scanner. Each specimen was scanned with a voltage of 120 kV, an

### Table 1

<table>
<thead>
<tr>
<th>Proportion of raw material [g/l]</th>
<th>X-mix</th>
<th>1A-mix</th>
<th>1B-mix</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blast furnace slag</td>
<td>604.9</td>
<td>314.2</td>
<td>377.7</td>
</tr>
<tr>
<td>CEM 42.5N</td>
<td>259.2</td>
<td>483.4</td>
<td>458.0</td>
</tr>
<tr>
<td>Silica fume</td>
<td>70.1</td>
<td>51.5</td>
<td>51.7</td>
</tr>
<tr>
<td>Limestone</td>
<td>864.1</td>
<td>446.6</td>
<td>194.7</td>
</tr>
<tr>
<td>Sand with grain sizes of 125–250 μm</td>
<td>283.6</td>
<td>286.3</td>
<td>263.4</td>
</tr>
<tr>
<td>Sand with grain sizes of 250–500 μm</td>
<td>345.6</td>
<td>347.0</td>
<td>355.0</td>
</tr>
<tr>
<td>Water</td>
<td>5.1</td>
<td>5.2</td>
<td>2.7</td>
</tr>
<tr>
<td>Viscosity modifier admixture (VMA)</td>
<td>17.3</td>
<td>3.5</td>
<td>2.7</td>
</tr>
<tr>
<td>Superplasticizer</td>
<td>26</td>
<td>26</td>
<td>26</td>
</tr>
</tbody>
</table>

### Table 2

<table>
<thead>
<tr>
<th>Volume percentage [%]</th>
<th>X-mix</th>
<th>1A-mix</th>
<th>1B-mix</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix</td>
<td>91.04</td>
<td>97.79</td>
<td>94.57</td>
</tr>
<tr>
<td>Fibre</td>
<td>0.04</td>
<td>0.03</td>
<td>0.02</td>
</tr>
<tr>
<td>Air voids</td>
<td>8.92</td>
<td>2.18</td>
<td>5.41</td>
</tr>
</tbody>
</table>

Fig. 7. Voxel density probability distributions of the X-mix (red), 1A-mix (green) and 1B-mix (blue), as obtained after contrast stretching and rescaling the density values between 0 and 1. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
amperage of 200 μA, and an open time of 500 ms. It was not possible to scan the entire specimen at a sufficiently high resolution, due to scanning equipment limitations of the X-ray detector of 2304 × 2304 pixels. The balance between voxel size and scanning volume led to a scanning resolution of 6.67 μm. This resulted in a 3D volume with a total size of 3.62 cm³, in correspondence with a voxel-to-volume ratio of 8.18 × 10⁻¹¹. The scanning procedure was performed by capturing an X-ray image every quarter of a degree under rotating the specimen with respect to the vertical axis (which corresponds to the longitudinal axis of the fibre), resulting in 1440 images of 2304 × 2304 pixels. With these images, a reconstruction of the 3D volume was made using VGSTUDIO software [36]. A 3 × 3 × 3 median filter was used over the entire 3D volume to reduce the noise while maintaining clear object edges.

The fibres in 3D printed SHCC practically never remain ideally straight, but rather show small curvatures [3]. Hence, there is a geometrical discrepancy between the straight fibre in the training specimen and the curved fibres in the 3D printed use-phase specimens. As described in Section 2.4, this problem was solved by selecting a sufficiently small window size within which the fibres of the 3D printed specimen appear as virtually straight, and the neural network could still accurately segment the three phases. For this purpose, a window size of 32 × 32 × 32 voxels (≈ 213.33 × 213.33 × 213.33 μm³) was selected. As explained, from the X-mix scan three different types of datasets were created that were characterized by a different directional bias of the yarn of fibre, i.e., the unidirectional, orthodirectional and omnidirectional datasets. By comparing the segmentation results calculated for these three datasets with those for the ground truth mask in Fig. 4(right), the effect of the proposed data augmentation procedure on the accuracy and convergence rate of the neural network result can be assessed.

The basic, unidirectional dataset was created by dividing both the ground truth mask and the cropped 3D volume into a batch of windows with a size of 32 × 32 × 32 voxels. The size of the first batch was limited to 90.0 × 10³ windows, which in the ground truth mask and cropped 3D volume were taken at equivalent locations. The spacing between the windows was set to 3 voxels in each direction. The orthodirectional dataset was augmented from the unidirectional dataset of the X-mix scan (90.0 × 10³ masks and 90.0 × 10³ windows from the cropped 3D volume) by considering 4 orthogonal fibre orientations (0°, 90°, −90°, 180°) along the 2 (positive and negative) directions of each of the 3 orthogonal coordinate axes, thus leading to the application of 4 × 2 × 3 = 24 orthogonal rotations to the 90.0 × 10³ windows, resulting in a total of 2160 × 10³ windows. Subsequently, the orthodirectional database was reduced to the same size as the unidirectional database, by arbitrarily selecting 90.0 × 10³ rotated windows from this set. In a similar fashion, an omnidirectional dataset of 90.0 × 10³ windows was created from the X-mix scan by applying the data augmentation procedure described in Section 2.4. Omnidirectional datasets were also created from the scans of the 1A-mix and 1B-mix specimens. Correspondingly, an initial window size of 56 × 56 × 56 voxels was selected that was subsequently cropped to 32 × 32 × 32 voxels after performing the fibre rotation operation, in accordance with the schematization presented in Fig. 5. Note that the edge length of the window is hereby determined as

\[ a = \sqrt{3b} = \sqrt{3 \times 32} = 55.4 \approx 56 \text{ voxels}. \]

Each of the three generated datasets was subsequently split in 80% training data (72.0 × 10³ windows) and 20% validation data (18.0 × 10³ windows). The training data were divided into batches of 64 windows with a size of 32 × 32 × 32 voxels, which resulted in 72.0 × 10³ / 64 = 1125 iterations per epoch. An issue that requires specific attention is the masking of the fibre cross-section. In principle, this is done by selecting the voxel that contains the central axis of the fibre in every 100th layer, followed by assigning a prescribed number of voxels around this centre voxel to construct the fibre mask. Since the fibre diameter of 40 μm corresponds to only 6 (square) 6.67 μm voxels, the transition zone of voxels containing both the fibre class and the matrix or air void class becomes relatively large. These ‘mixed phase voxels’ contaminate the mask, and actually should contain single-class information instead. Considering that the fibre mask width needs to be equal to an uneven number of voxels, i.e., the centre voxel plus, for symmetry reasons, an equal number of voxels at each side, the width and height of the fibre mask are set to correspond to 5 voxels. This results in two possible fibre mask configurations, designated in Fig. 9 as fibre mask type a and fibre mask type β.

As illustrated in Fig. 10, for both fibre mask types the centre of the circular fibre cross-section usually does not exactly coincide with the centre of the fibre mask. Specifically, as a result of the random distribution of fibres, relative shifts between the two centre points will arise in horizontal and vertical directions. The maximum value of this relative shift equals the half-width of a voxel, recalling that the fibre centre always falls within the central voxel of the fibre mask. Consider first the case whereby there is no relative shift between the cross-sectional centre of the fibre and the centre of the fibre mask, see Figs. 10(a) and (d). It can be observed that mask type a contains less fibre voxels (i.e., the dark green voxels) within the fibre circumference than mask type β, and thus automatically contains more matrix and/or air void voxels (i.e., the red voxels appearing within the fibre circumference). Since the training and validation of the neural network is based on the fibre ground truth mask instead of the circular fibre cross-section, it is important to realize that these red voxels will be interpreted as correct matrix or air void class predictions. Conversely, when the fibre mask experiences a maximal horizontal shift equal to the half-width of a voxel, see Figs. 10(b) and (e), or a maximal horizontal and vertical shift equal to the half-width of a voxel, see Figs. 10(c) and (f), one or more fibre mask voxels intersect with the outer circumference of the fibre (i.e., the light green voxels). In the most critical case depicted in Figs. 10(c) and (f), the dark green voxels of mask types a and β that entirely fit within the fibre circumference respectively relate to
Fig. 10. Various relative shifts of the fibre mask towards the fibre circumference, with the maximal, horizontal and vertical shifts equal to the half-width of a voxel. The fibre mask voxels intersecting with the fibre circumference are indicated in light green. (a) Mask type $\alpha$, no shift. (b) Mask type $\alpha$, maximal horizontal shift. (c) Mask type $\alpha$, maximal horizontal and vertical shift. (d) Mask type $\beta$, no shift. (e) Mask type $\beta$, maximal horizontal shift. (f) Mask type $\beta$, maximal horizontal and vertical shift. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Fig. 11. An illustrative example of a neural network prediction for a hypothetical fibrous composite, with (a) the ground truth mask of the micro-structure, which is composed of 80 (light grey) matrix voxels, 10 (dark grey) fibre voxels and 10 (black) air void voxels, and (b) the neural network prediction of the micro-structure, consisting of 75 (light grey) matrix voxels, 12 (dark grey) fibre voxels and 13 (black) air void voxels. The wrongly predicted voxels are indicated by the red dotted squares. The ‘overall accuracy’ of the prediction is determined by the total number of correctly predicted voxels of the three classes, and equals \( \frac{75 + 10 + 10}{100} \times 100\% = 95\% \). The ‘weighted accuracy’ of the prediction accounts for the size of each of the classes, and equals \( \left( \frac{75}{80} + \frac{10}{10} + \frac{10}{10} \right) \times 100\% = 97\%.9\% \).

\( \frac{12}{14} \times 100\% = 84.6\% \) and \( \frac{15}{21} \times 100\% = 71.4\% \) of the total cross-section of the corresponding fibre mask. In addition, for mask type $\alpha$ the most critical, light green, dotted-line voxels that cross the fibre circumference still fit within the circular fibre cross-section for 93%, while for mask type $\beta$ this is only 57%. From this comparison, it is expected that the prediction of the neural network with mask type $\alpha$ is more accurate than with mask type $\beta$. In Section 3.6 this hypothesis is validated by comparing the results calculated for both mask types using the omnidirectional dataset created from the X-mix.

The neural network calculations were performed on a node of the high-performance computing Linux server of the Eindhoven University of Technology, which features a 12 core Intel Xeon Gold 6128 CPU and a NVIDIA Tesla V100 16 GB GPU. For the performance of the simulations, primarily the calculation capacity of the GPU was utilized.

3.3. Interpretation and assessment of neural network calculations

Before discussing the results calculated by the neural network, in Fig. 11 an illustrative example is presented to explain how the results are interpreted and assessed. The hypothetical ground truth mask shown in Fig. 11(a) consists of 100 voxels in total, of which 80 (light grey) voxels are labelled as ‘matrix’, 10 (dark grey) voxels are labelled as ‘fibre’, and 10 (black) voxels are labelled as ‘air void’. The hypothetical prediction of the neural network is shown in Fig. 11(b), which illustrates that 75 voxels are correctly identified as ‘matrix’, and
also that all 10 fibre voxels and all 10 air void voxels are correctly identified. The correctly predicted voxels are commonly referred to as ‘true positives’. Hence, the ‘overall accuracy’ of the prediction equals \((75 \times 100\% + 80 \times 100\% + 80 \times 100\%) \div 3 \times 100\% = 95.0\%\), and the ‘weighted accuracy’, which accounts for the size of the object classes, equals \((75 \div 3 + 10 \div 3 + 10 \div 3) \times 100\% = 97.9\%\). The wrongly predicted voxels are designated in Fig. 11(b) by the red dotted squares, of which the two black voxels and the three dark grey voxels are ‘false positives’ for, respectively, the air void and fibre classes, and the sum of these 5 voxels represents the ‘false negatives’ for the matrix class. Class predictions as shown in Fig. 11(b) are typically determined by selecting for each voxel the class with the highest percentage prediction.

In addition to the overall and weighted accuracies, the ‘loss’ of the neural network can be determined by means of the so-called ‘categorical cross-entropy’ (CE), as defined by

\[
CE = -\sum_{i=1}^{n} y_i \log \hat{y}_i, \tag{1}
\]

where \(y_i\) is the target value of a specific voxel in the ground truth and \(\hat{y}_i\) is the value predicted by the neural network. For example, for a specific, single voxel the prediction by the neural network may correspond to class probabilities of 95% matrix, 4% fibre and 1% air void, which, with Eq. (1), leads to a categorical cross-entropy of \(CE = -(1 \times \log (0.95) + 0 \times \log (0.04) + 0 \times \log (0.01)) = 0.022\) for that voxel. After the categorical cross-entropy is determined for each voxel in the domain, the average value is computed by dividing the sum of all cross-entropies by the total number of voxels. Note that the categorical cross-entropy reaches the zero limit value if the class predictions of all voxels in the domain are in perfect agreement with those of the ground truth.

The ground truth and the corresponding prediction shown in Fig. 11 can be analysed in more detail by means of a so-called ‘confusion matrix’, see Fig. 12. In Fig. 12(a) the network segmentation result is summarized by presenting the predictions per class via percentual values measured with respect to the ground truth data. For example, for the class ‘matrix’, a total of 80 voxels is present in the ground truth mask; however, only 75 voxels are correctly predicted as ‘matrix’, in correspondence with a percentage of \(\frac{75}{80} \times 100\% = 93.75\%\) that appears in the left entry of the first row. For the remaining 5 voxels of the ‘matrix’ class, 3 voxels are predicted as ‘fibre’ and 2 voxels as ‘air void’, in correspondence with, respectively, percentages of \(\frac{3}{80} \times 100\% = 3.75\%\) and \(\frac{2}{80} \times 100\% = 2.50\%\) that appear in the middle and right entries of the first row. Clearly, the sum of the 3 entries of each row represents the ground truth of each specific class, and thus equals 100%.

Consider now, as a specific choice, the ‘matrix’ class. As illustrated in the qualitative representation in Fig. 12(b), the upper left (dark green) entry that relates to both the prediction and the ground truth of the matrix class indicates the ‘true positives’ (TP), while the 4 (light green) entries not related to the matrix class are the ‘true negatives’ (TN) of this class. Further, the 2 off-diagonal (red) entries related to the prediction of the matrix class are the ‘false positives’ (FP), while the 2 off-diagonal (red) terms related to the ground truth of the matrix class are the ‘false negatives’ (FN). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
characterizing the ground truth mask. Note that in the unfavourable situation of an ‘overfitting’ by the neural network its prediction would be characterized by a monotonic increase of both the weighted accuracy and the categorical cross-entropy, implying that the volume fractions of the three micro-scale objects become more accurate under an increasing number of epochs, but that the local class probabilities of the three micro-structural objects increasingly deviate from those of the ground truth mask. In summary, from the results in Fig. 13 it may be concluded that after 100 epochs the class predictions of training data and validation data for a unidirectional dataset almost perfectly match the class data defining the ground truth mask.

3.5. Training and validation of neural network using an orthodirectional dataset

Figs. 14(a) and 14(b) illustrate the overall and weighted accuracies and the categorical cross-entropy for, respectively, the training and validation of the neural network employing the orthodirectional dataset. The orthodirectional dataset was established from the single-fibre specimen configuration in Fig. 4 using the X-mix composition and fibre mask type $\alpha$ depicted in Fig. 9, and applying the data augmentation procedure with orthogonal orientation angles. Although both for the training data and validation data the trends for the overall accuracy and weighted accuracy are similar to those for the unidirectional dataset, the convergence rate is somewhat lower, leading to lower percentual accuracies at 100 epochs that lie between 99.0% and 99.5%. Recall that the total amount of data used in the unidirectional and orthogonal sets is the same, so that the lower convergence rate for the orthogonal training and validation sets can be explained from the fact that the amount of data in each of the orthogonal directions is lower than in the specific vertical direction solely considered in the unidirectional dataset. Further, despite that the categorical cross-entropy monotonically decreases with an increasing number of epochs, for the training data and validation data their values at 100 epochs equal 0.027 and 0.028, and thus still lie somewhat above zero. Hence, for an orthodirectional dataset the class predictions of training data and validation data capture the class data of the ground truth mask quite closely, but less accurate than for the unidirectional dataset.

3.6. Training and validation of neural network using an omnidirectional dataset

Figs. 15(a) and 15(b) show the overall and weighted accuracies and the categorical cross-entropy for respectively the training and validation of the neural network employing three different omnidirectional datasets. The three datasets were established from the single-fibre specimen configuration in Fig. 4 using the X-mix (red line), 1A-mix (green line) and 1B-mix (blue line) material compositions, in combination with the fibre mask type $\alpha$ depicted in Fig. 9 and the data augmentation procedure based on arbitrary fibre orientation angles. For the X-mix, the overall trends of the accuracies and categorical cross-entropy are consistent with those of the orthodirectional and unidirectional datasets presented in Figs. 13 and 14, respectively. However, the convergence rate under an increasing number of epochs is lower, due to the lower amount of data defining each specific fibre direction in the omnidirectional dataset. When comparing the individual results for the three mixes, it appears that the convergence rates for the X-mix and 1A-mix are comparable, leading after 100 epochs to overall and weighted accuracies of about 99%, and a categorical cross-entropy of 0.04. In contrast, the 1B-mix clearly has a lower convergence rate, which results after 100 epochs in overall and weighted accuracies for the training and validation datasets between 96.8% and 97.8%, and a categorical cross-entropy of approximately 0.08. In order to reach similar accuracy and cross-entropy values as found for the X- and 1A-mixes after 100 epochs, the number of epochs for the training of the 1B-mix had to be increased to approximately 2000. In the following, the neural network result calculated for the 1B-mix after 2000 epochs is compared to the results for the X-mix and the 1A-mix after 100 epochs, in order to ensure that the three networks have the same accuracy level.

For obtaining more detailed insight into the accuracy of the neural network calculations, the omnidirectional training datasets of the three mixes are used to predict the three specific phases in the single-fibre sample depicted Fig. 4, whereby the segmentation result computed for each mix is compared to the class ground truth data for that mix by means of a confusion matrix.

In Figs. 16(a) and 16(b) the class prediction for the X-mix is shown for the fibre mask types $\alpha$ and $\beta$ depicted in Fig. 9. For both fibre masks the diagonal terms of the confusion matrix indicate that the accuracy of the fibre prediction turns out to be the lowest of the three phases, followed by the predictions of the matrix material and the air voids. Specifically, for fibre mask type $\alpha$ the accuracy reaches an acceptable percentage of 92.5%, while for fibre mask type $\beta$ this percentage is significantly lower, namely 88.3%. The accuracies of the predictions of the matrix and air voids for both fibre mask types are significantly higher, between 98.5% and 99.8%. This result confirms the expectation that the fibre phase generally is the most difficult phase to segment. The false positive rate of the fibre class, as defined via Eq. (2), for the fibre mask types $\alpha$ and $\beta$ equals $\text{FPR}_{X,\alpha} = 0.005$ and $\text{FPR}_{X,\beta} = 0.005$, respectively. Both values are similar and very close to zero, indicating that the part of the fibre-reinforced sample that is predicted as ‘fibre’, indeed is very accurately predicted as ‘fibre’. Conversely, in accordance with Eq. (3), the false negative rates of the fibre class with mask types $\alpha$ and $\beta$ are $\text{FNR}_{X,\alpha} = 0.075$ and $\text{FNR}_{X,\beta} = 0.117$, respectively, which are significantly larger than zero.
thus indicating that many fibre parts in the actual fibre-reinforced sample are incorrectly predicted by the neural network. Most of the false negatives are found at the circumference of the fibre mask, at the transitions between the fibre and matrix/air voids, where certain voxels relate to more than one object class. In Fig. 10(b),(c) and Fig. 10(e),(f) these so-called ‘mixed phase voxels’ of the fibre masks $\alpha$ and $\beta$ are schematically indicated in light green. Observe from these figures that the mixed phase voxels for fibre mask type $\beta$ are larger in number than for mask type $\alpha$, which is in agreement with the higher value for the false negative rate calculated above. In summary, from the above comparison it may be generally concluded that fibre mask type $\alpha$ is preferential for the construction of the ground truth data set.

Figs. 17(a) and 17(b) respectively illustrate the class predictions for the 1A- and 1B-mixes, using fibre mask type $\alpha$. The accuracies of the fibre predictions are 78.1% and 83.1% for the 1A- and 1B mixes. As for the X-mix, the predictions of the matrix and air void phases in both mixes have a substantially higher accuracy, between 98.3% and 99.8%. With Eq. (2), the false positive rates for the fibre class in the 1A- and 1B-mixes are calculated as $\text{FPR}_{f,\alpha}^{1A} = 0.003$ and $\text{FPR}_{f,\alpha}^{1B} = 0.010$, respectively, which are close to zero and therefore acceptable. The false negative rates of the fibre class in the 1A- and 1B-mixes follow from Eq. (3) as $\text{FNR}_{f,\alpha}^{X} = 0.218$ and $\text{FNR}_{f,\alpha}^{1A} = 0.169$, respectively. When comparing these values with the value of $\text{FNR}_{f,\alpha}^{X} = 0.075$ calculated...
false predicted at locations at which, in principle, matrix material able to segment the fibre phase, although fibre parts frequently are X-mix composition. For the 1B-mix, the network prediction is well the network prediction of the fibre phase is most accurate for the absolute sense results in the incorrect prediction of a significant amount volume of matrix material present in the sample, and therefore in an be small, it should be realized that this percentage relates to the large percentage of 1.3% incorrect fibre prediction for the 1B-mix appears to larger than that for the 1A-mix (i.e., 0.3%, see Fig. 17(a)). Although a than that for the X-mix (i.e., 0.6%, see Fig. 16(a)) and more than 4 times the confusion matrix in Fig. 17(b), which is more than two times larger prediction is characterized by the relatively high percentage of 1.3% in locations at which the matrix actually should have appeared; this false observation is that for the 1B-mix the fibres frequently are predicted at are considerably lower, namely 8.1% and 5.1%. Another important comparison.

Fig. 17. Percentual class predictions for the single-fibre SHCC specimen, based on the omnidirectional dataset, and (a) the 1A-mix and mask type \(a\) (at 100 epochs), and (b) the 1B-mix and mask type \(a\) (at 2000 epochs). The class predictions are calculated with respect to the ground truth data.

In summary, from the above analysis it may be concluded that the fibre phase is predicted most accurately for the X-mix, followed by the 1B-mix, and finally the 1A-mix.

In Fig. 18 the ground truth mask of the single-fibre specimen for the three mixes is compared to the corresponding segmented micro-structure predicted by the neural network with fibre mask type \(a\). The figure has been deduced from a three-dimensional representation by displaying the cementitious matrix as transparent, and thus shows the air voids (depicted in grey) and fibre (depicted in red) in the depth direction of the sample. It can be confirmed that for all three mixes the predicted matrix and air void phases are in close agreement with those of the corresponding ground truth mask. This is indeed in line with the high percentual values (i.e., close to 100%) of the ‘air void’ and ‘matrix’ diagonal terms in the confusion matrices 16(a), 17(a) and 17(b) of the X-, 1A- and 1B-mixes. Observe further from Fig. 18 that the X-mix clearly has the largest amount of air voids, followed by the 1B-mix and finally the 1A-mix, in accordance with the volume percentages listed in Table 2. While the air voids in the X- and 1B-mixes locally have a relatively large size, in the 1A-mix the air voids typically are quite small. It can be further seen that for all three mixes the fibre thickness following from the neural network prediction is somewhat larger than in the corresponding ground truth mask. Hence, within and around the cross-section of the fibre mask shown in Figs. 10(a) to 10(c), not only the dark and light green voxels are identified as ‘fibre’, but also some of the red voxels. Observe further that the predicted fibre geometry for the 1A-mix illustrated in Fig. 18b shows several discontinuities in the longitudinal fibre direction that are occupied by matrix material. This erroneous result is illustrated in the confusion matrix of the 1A-mix by the high percentage of false matrix prediction of 16.4%, see Fig. 17(a). Indeed, the confusion matrices in Figs. 16(a) and 17(b) show that these percentages for the 1B-mix and the X-mix are considerably lower, namely 8.1% and 5.1%. Another important observation is that for the 1B-mix the fibres frequently are predicted at locations at which the matrix actually should have appeared; this false prediction is characterized by the relatively high percentage of 1.3% in the confusion matrix in Fig. 17(b), which is more than two times larger than that for the X-mix (i.e., 0.6%, see Fig. 16(a)) and more than 4 times larger than that for the 1A-mix (i.e., 0.3%, see Fig. 17(a)). Although a percentage of 1.3% incorrect fibre prediction for the 1B-mix appears to be small, it should be realized that this percentage relates to the large volume of matrix material present in the sample, and therefore in an absolute sense results in the incorrect prediction of a significant amount of fibre parts, see Fig. 18c.

In summary, from the above analysis it may be concluded that the network prediction of the fibre phase is most accurate for the X-mix composition. For the 1B-mix, the network prediction is well able to segment the fibre phase, although fibre parts frequently are falsely predicted at locations at which, in principle, matrix material should appear. Finally, for the 1A-mix the network prediction misses fibre parts along the longitudinal fibre direction, and at these locations falsely predicts the presence of matrix material.

3.7. Prediction of micro-structure of 3D printed use-phase specimen

A single SHCC use-phase specimen with randomly distributed and oriented PVA fibres was 3D printed at the Eindhoven University of Technology using the X-mix composition. The material was premixed before it was placed inside the second chamber of an M-tec duo-mix connect. This mixing device uses is a TMV 75 pan mixer fabricated by Van der Zalm Nuth B.V., and is characterized by a capacity of 75 litres, an engine power of 2.2 kW, and a single rotational speed. The material was extruded using a rotor-stator pump with a 5-metre hose connected to it. The printing nozzle had an opening of 40 × 14 mm². More details on the 3D printing process can be found in [2].

The \(\mu\)CT scanning procedure of the hardened use-phase specimen was performed with the settings outlined in Section 2.2. In order to assess the influence of the specific specimen characteristics used for the training of the neural network on its predictive capability for one and the same 3D printed sample, the segmentation prediction for the X-mix use-phase specimen is compared for neural networks trained on, respectively, the omnidirectional datasets of the X-mix, 1A-mix and 1B-mix. Note that the ground truth mask has not been established for the use-phase specimen, and thus cannot be incorporated in the comparison.

Fig. 19 shows a 3D image of the X-mix use-phase specimen, with the specimen geometry as obtained from the \(\mu\)CT scanning procedure illustrated at the bottom, and the phase segmentation predicted by the neural network trained on the X-mix shown at the top. Both the fibres (depicted in red) and the air voids (depicted in grey) are approximatively uniformly distributed across the specimen, and clearly occupy a significantly lower volume than the cementitious matrix (depicted as transparent). Note that the fibres show a slight orientation preference in (approximately) the vertical direction, which likely originates from the fibre mixing and layer extrusion process typical of the 3D printing procedure. Further, the geometry of the air voids varies across the specimen, with the overall sizes ranging from 0.2 mm to 6 mm in diameter. Finally, it can be observed that fibre clumping does not occur; essentially, in the case of fibre clumping the usability of the SHCC material would have been less, since the fibres then do not improve the mechanical performance of the composite. Additionally, it is difficult to segment individual fibres within a clump, as local voxel density differences vanish when fibres get into contact with each other.

Fig. 20 shows the top view of the fibrous composite micro-structure predicted by the three neural networks. The prediction from the neural network trained on the X-mix (Fig. 20(a)) is in good agreement with that from the neural network trained on the 1B-mix (Fig. 20(c)). The
respective fibre volume percentages are 2.67% and 2.69%, and slightly overestimate the average fibre volume percentage of 2% applied in the specimen preparation procedure. This overprediction is partly due to the fact that the use-phase specimen was cut at the centre of a printed layer, at which the fibre concentration seemed to be somewhat larger than at the layer boundaries. The air void predictions of the two mixes also appear to be reasonably close, in correspondence with volume percentages of 1.64% and 2.01%, respectively. In contrast, the calculation from the neural network trained on the 1A-mix (Fig. 20(b)) leads to a comparable air void percentage of 1.53%, but results in a very low fibre volume percentage of 0.05%. The relatively large false prediction of the fibre phase following from the network trained on the 1A-mix was also observed for the single-fibre specimen, see Section 3.6, although the effect here is much stronger. A possible explanation for this enhanced effect may be that the voxel density probability distributions of the X-mix use-phase specimen and the 1A-mix training specimen are significantly different, see Fig. 7. The figure further shows that the voxel density probability distribution of the 1B-mix training specimen is very close to that of the X-mix use-phase specimen, which, together with the observation that the 1B-mix trained network is well capable to segment the fibre phase, see Section 3.6, indeed may be the reason that the phase segmentation calculated by the neural network trained on the 1B-mix is in good correspondence with that trained on the X-mix, see Figs. 20(c) and 20(a).

In order to further explore the relatively large sensitivity of the 1A-mix trained network for underpredicting the fibre phase and to check the network robustness, (i) the selection criterion used for identifying the fibre class during the network training has been varied by reducing the threshold value for the fibre class to 0.1, and (ii) the omnidirectional datasets used for the training process have been varied by generating a different random selection of fibre orientations in the data augmentation procedure. A reduction of the threshold value for fibre identification to 0.1 means that a voxel will be labelled as ‘fibre’ if the accuracy of the network prediction is 10% or larger. In comparison with

![Fig. 18. Segmented micro-structure for the single-fibre SHCC specimen according to the ground truth mask (left) and the neural network prediction (right) that uses fibre mask \( \alpha \) and the omnidirectional dataset, for (a) the X-mix (prediction at 100 epochs), (b) the 1A-mix (prediction at 100 epochs) and (c) the 1B-mix (prediction at 2000 epochs). The fibre is designated in red, the air voids in grey, and the cementitious matrix is displayed as transparent. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)](#)
The automated image segmentation method has been applied to a strain-hardening cementitious composite (SHCC) composed of a cementitious matrix reinforced with polystyrene fibres. The training and validation of the network has been performed by using three single-fibre specimens with a different SHCC mix design. The mix designs were taken from the literature, and were developed for 3D concrete printing applications. For one of the mix designs (X-mix), the neural network has been trained and validated for three different selections of fibre orientations, namely a unidirectional set (fibres oriented in one specific direction), an orthodirectional dataset (fibres oriented in three mutually orthogonal directions) and an omnidirectional dataset (fibres oriented in arbitrary directions). The comparison of the training and validation of the network for these three datasets has clarified for the single-fibre specimen how the selection of fibre orientations influences the accuracy and corresponding convergence rate of the network. Additionally, all three mix designs have been trained and validated by means of an omnidirectional dataset, after which a comparison study has illustrated the sensitivity of the network performance on the specific mix design applied. Subsequently, the predictive capability of the networks trained on the three mix designs has been demonstrated for an SHCC use-phase specimen that contains a large number of randomly distributed and oriented PVA fibres. The main conclusions of the experimental–numerical study are point-wisely summarized below.

- The automated image segmentation method appears to be very suitable for the efficient identification of complex micro-structures typical of a practical, fibre-reinforced composite material.
- The proposed data augmentation procedure proves to be an efficient tool for extending training data obtained from a single-fibre specimen for applications on samples containing a large number of arbitrarily distributed and oriented fibres.
- The convergence rate of the accuracy level of the neural network during training strongly depends on the composition of the data manifold. For fibrous composites in which the fibres are oriented in one specific direction, a data manifold based on arbitrary fibre orientations converges substantially slower than a data manifold based on the specific, single fibre orientation. Nonetheless, it is recommended to generalize the data manifold for arbitrary fibre orientations in order to broaden the applicability of the trained neural network.
- The accuracy of the micro-structure predicted by the neural network seems to strongly depend on the resemblance in the voxel density probability distributions of the fibrous composites selected for network training and network prediction. A significant difference in these voxel density probability distributions may lead to an inaccurate segmentation result for the fibre phase. The predictions of the matrix and air void phases are less sensitive for such differences.
- For the studied SHCC use-phase sample, which contains a large number of arbitrarily distributed and oriented fibres, changes in the fibre segmentation criterion and in the random selection of fibre orientations used for the data augmentation procedure only have a small to negligible effect on the specific micro-structure predicted by the neural network. In other words, the neural network behaves rather robustly under specific setting alterations applied during training.

The findings of the present study are of specific interest for the research field of 3D printing of strain-hardening cementitious composites, as it allows for the analysis of their mechanical properties based on detailed input of the actual fibrous composite micro-structure. To this date, this input has been virtually impossible to generate, due to the enormous effort involved in the manual segmentation of µCT-scanning data required for the training of a neural network. Moreover, the developed method provides new opportunities for the detailed micro-structural identification and analysis of other fibre-reinforced composites, such as fibre-reinforced plastics.
Fig. 20. Segmented micro-structure for the 3D printed SHCC use-phase specimen with an X-mix matrix, with the fibres designated in red, the air voids in grey, and the cementitious matrix displayed as transparent. Prediction by (a) an X-mix trained network, (b) a 1A-mix trained network, and (c) a 1B-mix trained network. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

CRedit authorship contribution statement

K. Nefs: Conceived and developed the methodology, Performed the experiments and simulations, Writing – original draft. V. Menkovski: Conceived and developed the methodology, Reviewed the manuscript. F.P. Bos: Conceived and developed the methodology, Reviewed the manuscript. A.S.J. Suiker: Conceived and developed the methodology, Writing – original draft. T.A.M. Salet: Conceived and developed the methodology, Reviewed the manuscript.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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