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Improving surface finish quality in extrusion-based 3D concrete printing using machine learning-based extrudate geometry control

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Abstract

3D Concrete Printing (3DCP) has been gaining popularity in the past decade. Due to the nature of layer-by-layer printing and the slump of the material deposition in each extruded lines, 3D printed structures exhibit obvious lines or marks at the layer interface, which affects surface finish quality and the lines are the potential crack initiation because of the stress concentration. This brings a necessity to control the extrudate formation in some critical applications. However, the formation of the extrudate's shape depends to a ton of factors, which make the direct analytical approach complex.

In this paper, a machine learning technique is applied to correlate the formation of the extrudate to the nozzle geometry and printing parameters using an Artificial Neural Network (ANN) model. The training data for the model development was obtained from printed extrudates using the 3DCP process with various printing parameters. Additionally, the performance of the trained model was validated using separate experiment. The extrudate geometry which was predicted by the model demonstrated good agreement with the experiment results. Subsequently, the developed model was used to evaluate a proper nozzle shape to produce a designated extrudate formation. Significant improvement on the printing quality was demonstrated using geometrically optimized nozzles generated from the model on 3D printed objects consisting a vertical wall, an inclined wall and a curved part.

1. Introduction

The 3D-printing technology, which is also referred to as additive manufacturing, is a fast-growing technology which is developed towards many engineering disciplines, ranging from polymer, metal, up to bio-printing applications. The 3D printing technology was also introduced into construction industry since Khoshnevis et al. developed the first 3D Concrete Printing (3DCP) process in mid-1990s [1]. Owing to the simplicity in directly creating specific shapes of concrete elements without the need of underlying formwork, the 3DCP can improve the total fabrication time and the labor cost in construction industry. As a result, a rapid development in 3DCP was seen and many studies [1-10] have shown full-scale printing with 3D Concrete Printing (3DCP) solutions. The increase in automation level of the approach and the decrease in labor cost has been noticeably observed [8, 11] .

Despite the rapid development, the lack of control in the geometrical shape of the extrudate limits the quality of 3DCP products. The extruded geometry deviates in the experiment and not necessarily follows the shape of nozzle outlet. This leads to a surface quality problem such as the jagged surface or staircase effect on the 3DCP product (see Fig. 1). Although many extrusion-based 3D printing processes have limited quality control [12-14] due to the material deformation [1, 15] or staircase effect [16], the surface roughness problem becomes too obvious to overlook in 3DCP because of the size of extrudate increases for large-scale printing. Rough surface finish tends to make the structure less robust to wearing than smooth surface [12, 17-19]. In addition to the surface quality, stress concentration at layer interface might reduce the layer bonding between the layers [20]. Therefore, it is very important to predict and control the surface roughness of the 3DCP-printed structure. Many experiment parameters, including the nozzle outlet shape, material flow rate, nozzle travel speed, nozzle standoff distance, and rheological performance of material could significantly influence the extrudate formation.

Many researchers currently focus on controlling the deposited extrudate geometry for vertical-wall printing. The Contour Crafting method [21, 22] employs trowels to comb any excessive material directly, thus to ensure rectangularity of the extrudate geometry. Kwon et al. concluded that modifying the nozzle outlet shapes will influence the extrudate geometry [23]. It is also concluded that the rheological property of the deposited material noticeably affect the deviation of the extrudate nominal geometry as presented by Roussel in [11]. However, these efforts didn't focus on the control of final geometrical dimension of extrudate. The lack of

control on the extrudate geometry constrains the further improvement on the surface finish quality, especially for parts with complex curvatures. For example, the dome printed by Contour Crafting [24] shown in Fig. 1(b) still exhibits obvious staircase effect.

Fig. 1: (a) Jagged surface on the vertical wall printed by TU/e and (b) staircase effect on the miniature dome printed by contour-crafting

The ability to direct control the extrudate geometry will allow the creation of smooth wall surface for complex product in 3DCP. As an illustration, the inclined wall in Fig. 2a will have a smooth surface finish only if the geometry of the extrudate in every layer can be controlled to have a slanted outer side, thus having a trapezoid-like extrudate geometry in each layer. Otherwise, the printed part would exhibit staircase-like wall illustrated in Fig. 2(b-c), which can reach up to several millimeters width [25]. The width of the ridge in the staircase-like wall is fully dependent to the nozzle size which might vary from 10 mm to 40 mm in 3DCP [26]. In small scale printing like FDM, this staircase problem is typically improved by using a smaller nozzle size or reducing layer height [16]. However, reducing the nozzle size is not practical in large-scale extrusion printing like 3DCP due to the long printing time for large concrete structures. Therefore, applying direct control to extrudate geometry seems to be a more promising way to improve surface finish quality without compromising the printing speed.

Fig. 2: Staircase effect in 3D printed parts: (a)The design of the object, (b) the sliced layer-by-layer model and (c) the staircase effect

To control the extrudate geometry, development of a reliable predictive model is needed that can estimate the final geometrical dimension of the extrudate as a function of the printing parameters, including the nozzle shape, rheological properties of material and flow rate. Analytical modelling of the relationship between the extrudate geometry and the printing parameters is too complex. Apart from the numbers of affecting parameters, the 3D printing process is a three-dimensional case, which makes the analytical solution nearly impossible. The computational fluid dynamics (CFD) simulation have been used to predict the deformation of extrudate during the extrusion-based deposition of molten ceramics and polymers [23, 27, 28] and analyze the flow problem of concrete [29-31]. However, the simulation approach for the 3DCP problem involves the interaction of two different phases (air phase and cementitious

material phase), and it involves a moving boundary-condition problem because of the nozzle movement during the deposition. Therefore, applying the simulation methodology with CFD approach is very time-consuming. Moreover, the simulation approach will require the establishment of an extensive database, which consists of many different configurations of extrudate formation and the corresponding boundary conditions, to achieve the goal of controlling the extrudate geometry. Therefore, using the simulation approach to create a controller for extrudate geometry is impractical.

Machine learning technique is seen to be an alternative to develop predictive model for concrete extrudate geometry. The basic idea of a machine learning approach is to train a model to recognize the pattern from the training dataset that correlates the input parameters and the extrudate geometry as the output state, which subsequently, the model can be used to predict the output for any given input entities. The artificial neural network (ANN) is a computational implementation of the machine learning technique, which is capable of developing a predictive model directly by feeding a proper training data. This machine learning method has been proven to be useful in many areas, including hand-writing classification, speech recognition, image classification [32-34]. There is a new trend to introduce machine learning to 3DCP-related areas [35]. The machine learning method has been introduced to 3D printing process to predict extrudate formation process and surface roughness [12, 19, 36], and also the prediction of the flowability and mechanical strength of concrete [37-41]. The trained ANN model could instantly predict the extrudate geometry after being trained with proper experiment data. Therefore, in this paper, the machine learning method is used to develop a predictive model for extrudate geometry in 3DCP.

This study aims to present a novel approach to directly control the geometrical dimension of extrudate in 3DCP. A predictive model for extrudate geometry is developed based on machine learning method and the model can be subsequently used as a basis to improve the quality of the printed product. In section 2, the parameters affecting extrudate deformation are discussed and the modelling strategy is explained. In section 3, the experiment setup for acquiring training dataset is introduced. In section 4, a predictive ANN model was trained based on 3DCP experiment data and the model architecture was optimized. The experimental validation shows the capability of the developed model to accurately predict extrudate geometry. Furthermore, the model is suitable to instantly predict nozzle shapes which can be used to print extrudate with different target geometries and improve printing quality for 3DCP

parts with desired surface curvatures. With this approach, the extrudate geometry can be simply controlled in the 3DCP process and the printing quality can be improved for structures even for surface curvatures more complex than normal vertical-wall printing.

2. Research Methodology

2.1. Description of extrudate deformation in printing process

The extrusion-based 3D printing process is initiated by pumping the material through the pipe to the printing head or nozzle. Simultaneously, the printing head is repositioned following the designated trajectory of the printed wall to deposit the extruded material layer-by-layer. The mixture ingredients and mixing code significantly affect the behavior of the material [42-44]. Roussel in [11] explicitly presented the requirement of printable materials, where the material should be sufficiently flowable to be pumped through the pipe, yet it should be stiff enough to retain the shape and to sustain its weight. However, as the fresh state material has to be pumpable and flowable, the extruded material in one layer tends to slump and deform immediately after it is deposited. This deformation often increases when additional layers are placed on top due to the weight and force exerted on lower layers.

Theoretically, the final geometry of the extrudate can be calculated analytically from the material flow during the deposition. The printed cementitious material can be assumed as a single-phase non-Newtonian fluid and the flow behavior of material follows the Navier-Stokes equations because the flow channel has a much larger dimension than the particles [45].

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1)$$

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} \quad (2)$$

$$\boldsymbol{\tau} = \tau_0 + k\dot{\gamma} \quad (3)$$

In the 3DCP extrusion process, the material will finally stop flowing and reach a final steady state and exhibits the final geometry. The final state of the flow can be calculated with the governing equations Eqs. (1)-(3) and the boundary conditions C .

The final geometry of the extrudate (E) can be obtained from the final state of the flow F . Therefore, we can assume a functional relationship f exists between the final flow state F and a set of flow boundary conditions (C), which represent the printing parameters in the 3DCP experiments. So, the final extrudate geometry can also be obtained as Eqs. (4).

$$\mathbf{E} = f(\mathbf{C}) \quad (4)$$

Before modeling the functional relationship f , the experiment parameters affecting the boundary condition C needs to be determined. These parameters might include the shape of the nozzle outlet, shape of the nozzle channel, the nozzle feed rate, the material flow rate, rheological properties of the material, etc.

The shape of nozzle outlet has a dominant effect on the geometry of the extrudate. The shape of nozzle outlet (D) will predetermine the shape of material just before the extrusion, which essentially is the initial extrudate shape before it is further deformed by any other factors discussed before. The material used in the printing is considered to be viscous fluid with Reynold number less than 1, in such the deformation of the material after leaving the nozzle will not be too excessive. In order to have a desired extrudate geometry, the shape of nozzle outlet needs to be adjusted, where most of rectangular-shaped nozzles used reported in many literature produce extrudate with almost-rectangular geometry [4, 22, 46].

The “localized” volume flow rate of the material, ε , is another vital factor, which is defined as a ratio between the material volume flow rate (Q) to the ideal material deposition rate:

$$\varepsilon = \frac{Q}{v_t * A} \quad (5)$$

An ideal material deposition rate is affected by nozzle feed rate (v_t) and the nozzle outlet area (A). When the localized volume flow ratio is less than 1, the material flow rate cannot match the deposition rate, which might result in underflow. On the contrary, when the localized volume flow ratio is greater than 1, the material flow rate is higher than the deposition rate, and overflow might happen [47]. Theoretically, any variations in the localized material flow rate will lead to different extrudate geometry. If severe overflow or underflow happens, the final extrudate geometry will be much harder to predict.

It is obvious that the rheological properties of material have a significant effect on the final geometry of extrudate. The dynamic yield stress corresponds to the deflocculated microstructure, which could affect the pumpability and flow rate. The dynamic yield stress also affects the process for the deposited material to stop flowing and build up strength [48]. On the other hand, the static yield stress is a rheological parameter that affects the geometric stability of extrudate in the individual strength-based layer and collective strength-based layer [11]. The concrete material exhibits different yield stress at static state because of particle flocculation [34] [49, 50]. The deposited material at static state is subjected to gravity shear force caused by its own weight and the weight of subsequent-deposited layers. If the shear force exceeds the static yield stress, the extrudate will slump and expand in width. If the shear force does not exceed the static yield stress, the material may still be exposed to an elastic deformation that is dependent to the elastic modulus (G). Thus, from rheological perspective of cementitious materials, the 3D printable materials should have low dynamic yield stress and high static yield stress and modulus.

Based on the previous discussion, the extrudate geometry is affected by several empirical parameters, including the nozzle shape (D), localized material flow rate (ε), dynamic yield stress (τ_D), static yield stress (τ_s) and elastic modulus (G), as represented mathematically as:

$$f(D, \varepsilon, \tau_D, \tau_s, G) = E \quad (6)$$

While the dynamic and static yield stresses and elastic modulus are tagged as material properties, this study aims at proving the concept of the predictive model with more focus on the effect of the nozzle design and the localized material flow rate. In short, in this study, only one type of mixture and material is used with an assumption that the rheological change during the deposition process is negligible. With the aforementioned assumptions, the parameters related to material properties are not considered in the developed model and will be studied in successive work. Therefore, the proposed model is simplified to be subjected to nozzle shape and localized flow rate:

$$f(D, \varepsilon) = E \quad (7)$$

In this model, we assume that a slight change in the boundary condition will only lead to a minimum change in the extrudate cross-sectional shape due to the high viscosity and low velocity of the deposited concrete material during the 3DCP process ($Re < 1$). A machine learning technique is chosen to be used to model the relationship due to the capability of

capturing complex nonlinear behaviour. It has to be underline, however, that the performance of the machine learning model is dependent to the data fed in the training process.

2.2. Machine learning

A typical structure of ANN consists of input layers, output layers and several hidden layers. Controllable variables, in our case is printing parameters, is fed to the input layer and subsequently, process the information through the hidden layers and finally represent the output, in this case is the predicted extrudate geometry, in the output layer. Each layer might be represented by many neurons, where each neuron comprises a weightage and a specific bias. The information is transmitted from one neuron to another neuron in the subsequent layer by edges, which means that each neuron can affect all the neurons in the next layer [51], iteratively until it reaches the output layer. By properly tuning the weightage and bias in all neurons, the overall network will represent the model that correlate the input and output entities.

Fig. 3: Schematic of a typical ANN model

In order to tune all the parameters in the ANN, the training dataset comprising the input data and the corresponding output data is needed. In our case, the input data are the printing parameters, while the observed extrudate geometries obtained from printing experiment represent the output. To highlight it again, as have been discussed in Section 2.1, the

rheological property of the material is kept fixed in the experiment, in such, only the shape of the nozzle outlet and material overflow ratio are considered as the input set for the ANN model.

Using all the training dataset, the model is subsequently optimized by tuning all the weight and bias of all the neurons upon the minimization of the errors between the prediction and the target. Often, the mean-square error (MSE) provides an adequate measure of prediction error and can be written as:

$$\text{MSE} = \sum_{i=1}^N \frac{(Y_i - \hat{Y}_i)^2}{(N)}$$

where Y_i is the target output in the training dataset, $\hat{Y}_i$ is the predicted output and N is the number of observations in the training set. The parameter optimization in the training step typically utilizes a back-propagation mechanism. At the initial stage, a random set of weightage and bias parameters are assigned to all the neurons, and the error between the computed output and actual output is calculated, where the parameters are adjusted in a backward sequence, from the last layer to the starting layer to reduce the error using an optimization algorithm. The optimum set of parameters, comprising the weight bias for every neuron is recorded once the optimization is finished. Upon a successful completion of the training process, the model will be ready and it will be able to predict the extrudate geometry output for any given input parameters.

After the predictive model is obtained, the nozzle shape can be obtained to print the targeted extrudate cross-sectional shape in experiments. While the ANN model can effectively predict the extrudate cross-sectional shape, it cannot be directly reversed because it involves the inversion of a non-square matrix, which cannot be accurately performed numerically. As a result, a nozzle-extrudate database was established to correlate the nozzle shapes and corresponding predicted extrudate cross-sectional shapes for inversely search nozzle shape from targeted extrudate cross-sectional shape. With this method, the extrudate formation can be controlled and the surface finish quality can be improved in 3DCP.

A summary of the workflow is illustrated in Fig. 4. The training data for the ANN model was gathered in pre-testing step. The predictive ANN model is then trained after topology optimization. With the predictive model, a database is established by connecting randomly generated nozzle shapes with their predicted extrudate cross-sectional shapes. Finally, nozzles

for different target extrudate cross-sectional shapes can be obtained from the database and used in the printing.

Fig. 4: The workflow to find the corresponding nozzle shape based on the expected extrudate formation

3. Experiment

3.1. Materials and experiment setup

The material used in the experiments was proposed in the work of Weng et al. [44] to meet the flowability and buildability requirement for printing. The material was composed of Portland cement, fly ash, sand, and water.

A Hobart mixer X200l was used for material mixing. The mixing procedures were fixed for the material in this study to ensure the consistency of rheology performance for different batch of material. The dry ingredients including cement, flow ash and sand were first weighted and mixed for 2 minutes under stir speed. Then, water was then added and mixed for 3 minutes under stir speed; and then, superplasticizer was then dosed to the mixture mixed for 2 minutes in stir speed and 2 minutes in speed I. Each batch of material was 6 liters.

The experiment setup used in the printing process is illustrated in Fig. 5. The gantry-typed printer used in the experiment has a printing volume of 1.2 m (L) × 1.2 m (W) × 0.8 m (H) and it was controlled by a traditional CNC controller. The gantry comprises four degrees-of

freedom (DOF), in addition to three displacement DOFs in x , y , and z directions and one rotational DOF R_x -axis. The gantry served as a motion system to move the nozzle along the printing trajectory following the input G-code. A pumping device (MAI Pictor pump) equipped with a delivery hose was used to deliver the cementitious materials during the printing through an auger screw mechanism. Both the print speed and the pump's speed were fixed after initial adjustment. Nozzles with pre-designed outlet shapes were fabricated by FDM printer Ultimaker 2 and mounted on the gantry to conduct the printing.

Fig. 5: Experiment setup for 3DCP including (a) the pump and gantry printer, (b) the material deposition nozzle and (c) the changeable nozzle outlet

To acquire training dataset to develop the relationship between the nozzle shape and extrudate geometrical dimension, 13 different shapes of nozzle outlet were considered, as depicted in Fig. 6. The top and bottom sides of the nozzle outlet were kept parallel and the distance between the top and bottom sides are held at 15 millimeters, as we considered the same stacking in each layer of extrudate deposition. These shapes were varied on the sides only, taking into account for different slopes with different angles, concavities and convexities, and asymmetries. The

cross-sectional area of the outlets, however, was maintained to be 450 square millimeters for all nozzle shapes, implying the same localized volume flow rate of the material. The bar on the nozzle represent the front side of the nozzle's moving direction in the printing.

Fig. 6: The 3D CAD model of nozzle, and 13 different shapes of nozzle used in the experiment. Note the bar on the nozzle design indicate the front side of nozzle movement.

3.2.Photo processing and data analysis

For every nozzle, a 500 mm long oval trajectory were printed with three layers. The two straight sections of the oval shape were parallel and printed along y axis, as illustrated in Fig. 7. After 7 days' curing, the straight-line section was cut into 40 mm length samples by a Struers Secotom-15 diamond cutter for further extrude shape analysis. It has to be noted that only the middle layer was used to for the training as the geometry of the bottom layer was affected by the printing board tilt, while the top layer was scratched by the nozzle. After each printing, the middle line of the printing path was also labeled on each sample by a needle for further analysis of the extrudate formation.

Fig. 7: (a) The 3-layer printing trajectory and (b) the cross-sectional shape of the printed sample

The extrudate cross-sectional shape was analyzed by reading the cross-section images with MATLAB image toolbox. Each image was acquired in a controlled illumination environment to minimize any possible shade and by keeping the camera perpendicular to the sample at a fixed distance, where the result is illustrated as shown in Fig. 7. The resolution and image size were kept fixed at 3024×3024 pixels and $200 \text{ mm} \times 200 \text{ mm}$.

To quantify the shapes of the extrudate cross-section and the nozzle outlet for modelling purpose, finite sample points on shape contour [52] were used. The nozzle design and extrudate cross-sectional shape were sliced into five sections horizontally, which result in twelve sample points for both sides. The sample points of nozzle design were represented as $D_1, D_2, \dots$, and D_{12} , while the samples of extrudate cross-sectional area were denoted as $E_1, E_2, \dots$, and E_{12} , as illustrated in Fig. 8. In this way, the input and target for the ANN model can be represented numerically.

Fig. 8: (a) Schematic of sample points in (b) nozzle design and (c) extrudate cross-section

In order to take the material flow effect on the model, the ratio of the extrudate cross-sectional area to that of the nozzle is calculated, where the extrudate area was measured by calculating the number of pixels on the cross-section and the nozzle shape was measured from the CAD software. A higher ratio, which later is referred to as the overflow ratio, implies that the material feed rate is high for the print speed and the material is overflowing.

From the experiment, it is noticed that the overflow ratio from the 101 samples inherently varies as presented in Fig. 9. This results in the variation of the overflow ratio from 1.05 to 1.35, although the motor pump voltage and the material composition were kept fixed on all 101 samples printed. The variation of the overflow ratio might be pertaining to the pumping

mechanism or the non-Newtonian nature of the printed material as it is known that the viscosity of concrete depends to the shear stress that might fluctuate during the printing process.

Fig. 9: Overflow ratio measured for all the tested samples

3.3.ANN model training

An ANN model was, subsequently, trained to correlate the resulting extrudate cross-sectional shape and the nozzle shape including the overflow ratio. For the back-propagation, the Levenberg-Marquardt method was used, where the training was carried out under MATLAB environment with Neural Network Toolbox. The input layer of the ANN network consists of 13 neurons that include the 12 sample points of the nozzle shape and the overflow ratio, where the target layer was 12 sample points of the extrudate cross-sectional shape. From the entire training dataset, 70% was used for training purpose, 15% was used for testing, while 15% was used for validation. The data used for these processes were randomly chosen by MATLAB.

The structure of the ANN model was optimized to improve the accuracy of the trained model. To evaluate the performance of different ANN architecture in the model accuracy, various numbers of hidden layers and neurons were tested in the trial-and-error process. The number of hidden layers in the ANN model was limited to 2 in the optimization process because the ANN model with two hidden layers could theoretically approximate any smooth mapping to any accuracy as stated by Heaton et al. [53].

To minimize the possibility of falling in local minima, 100,000 ANN models were independently trained with random initial seeds assigned by MATLAB. Upon the training of each model, the performance of the training, testing and validation sets were calculated by means of MSE. Finally, the ANN model with the best testing performance (smallest MSE) was found and recorded.

3.4. Database generation

From the optimized model, we expect to predict what the extrudate geometry will look like for a specific shape of nozzle outlet. However, in real application, we need to determine the optimal nozzle shape for a desired extrudate geometry. Unfortunately, it is observed that the model exhibits a non-invertible relationship, where different nozzle shapes might result in a same extrudate geometry.

To overcome the problem, a database was generated to record nozzle shapes which would be relevant to print selective extrudate cross-sectional shapes. Random, yet realistic, nozzle shapes were generated by varying the value of nozzle sample points between 12 to 18 mm while maintaining the nozzle cross-sectional area to 450 mm². However, to avoid unrealistic shape, the randomly generated nozzles were checked in two steps. Nozzles that comprise sharp angle features will be discarded as this shape as those with sharp angles, as illustrated in Fig. 10, could lead to severe discontinuities in material flow during printing. To filter such shapes, a MATLAB code to examine the geometry was generated and used.

Fig. 10: Sharp angle feature that might cause flow discontinuities on generated nozzle shapes

The second check in preparing the database is by controlling the overflow ratio. Ideally, the ratio between the area of predicted extrudate shape and the area of nozzle shape should correspond to the input overflow ratio. If the calculated ratio does not match the predetermined overflow ratio, the generated nozzle shape will be rejected. A MATLAB script was also written to filter such cases.

Subsequently, the remaining generated nozzles were fed to the predictive ANN model and a corresponding extrudate cross-sectional shapes were generated. The database was, subsequently, established by iteratively generate random nozzle shapes and recorded all the resulting extrudate shapes.

With the aid of the database, an appropriate nozzle shape can be evaluated for a desired extrudate cross-sectional shape. However, preceding the deployment of the algorithm for wall printing, a CAD model of the wall geometry should be analyzed. The wall model is sliced into layers, after which the target extrudate cross-sectional shape will be analyzed for each layer. Referring to the generated database, the relevant nozzle shape can be evaluated and used for printing of each extrudate layer.

3.5. Surface roughness factor

The surface roughness parameter was used to characterize the surface finish quality when a nozzle generated by ANN model was utilized in the printing. Owing to the common arithmetic average roughness, Ra , the same roughness measure is used in this study to quantify the surface finish quality of a wall printed product. The Ra was calculated based on the horizontal deviations between the expected outer-surface curvature and the actual measured profile. Unlike the Ra used in machining field, the surface deviation of wall printing product might reach up to several millimeters.

To characterize the improvement of surface roughness, the 3DCP printed structures were sliced and the cross-sectional image were used to analyze the surface quality. The profile was represented by a set of data points with 0.01 mm resolution. Subsequently, the profile is compared to the desired surface and the Ra was calculated as the arithmetical mean of the horizontal deviations between the all sample points on target surface profile and the measured profile.

4. Results

4.1. Extrudate slump behavior

From the experiment, 101 extrudate cross-sectional samples were generated, where some of them are illustrated in Fig. 11. The training dataset was established based on the geometrical samples, the corresponding nozzles shapes and the measured material overflow ratio.

Fig. 11: The 101 extrudate cross-section samples

The results show that the nozzle shape significantly affects the extrudate formation as illustrated by some samples shown in Fig. 12. Changing the slope on the two sides of the nozzle is shown to be effective to modify the final extrudate formation.

Fig. 12: Different nozzle outlet shapes lead to variation in the slump behavior of corresponding extrudate shapes: (a, c, d) Different nozzle outlet shapes; (b, d, f) corresponding extrudate cross-sectional shapes

4.2.ANN model training

The topology of the ANN model was optimized by trial-and-error. The performance of the ANN topology was tested for all the possible neuron configurations in two hidden layer

configuration. The maximum number of neurons in each hidden layer is limited to 20. For the first and second hidden layers, the neuron number was varied from 1-20. The ANN configurations include that without second layer is tested, thus only one hidden layer is present in the ANN model structure.

Each neuron configuration was trained 1,000 times with different initial seed and the most optimized parameters in terms of the testing performance (MSE) was recorded to be used as the final ANN model. The final ANN model consists of a single-hidden-layer and 5-neurons topology as shown in Fig. 13 with MSE of 0.2816. The model exhibited fast convergence, while the predicted output and the target in all datasets showed a satisfactory correlation ($R>0.999$) as indicated in Fig. 14.

Fig. 13: Optimized ANN structure

Fig. 14: The training performance and the regression of the ANN model

4.3.Validation of the trained model

The accuracy of the ANN model, subsequently, was revalidated by three test nozzles, which have different shapes than those in the training set. The designated test nozzles were fabricated and subsequently used to print some samples. The geometry of the extrudate samples were, therefore, analyzed and compared with the predicted extrudate shapes from the trained model. The results were compared and contrasted as shown in Fig. 15, where the blue dot lines indicate the experimentally-acquired extrudate geometries, while the red lines represent the predicted extrudate cross-sectional shapes from the trained model.

The mean prediction errors, which represent the average of the absolute difference between the experimental extrudate geometry and the predicted results, are 0.44 mm, 0.54 mm, and 0.58 mm for the three test nozzles a, b, and c, respectively. For 3DCP process, the prediction error of around 0.5 mm is still tolerable considering the average size of wall structures. Therefore, it concluded the three validations and the model is considered to be able to predict extrudate formations.

Fig. 15: (a, b, c) The shape of the three randomly generated validation nozzles and (d, e, f) the comparison between the extrudate cross-sectional shape measured in the experiment and predicted by the ANN model for validation nozzles

4.4. Sensitivity of the input parameter

After validation, in the first place, the influence of the overflow ratio to the extrudate geometry predictions were analyzed. Fig. 16 shows the predicted extrudate geometries as results from a fixed rectangular nozzle outlet shape, while the overflow ratio varied from 1.05 to 1.4.

As can be observed from Fig. 16, when the overflow ratio increases, the width of the predicted extrudate geometry also increases. It is observed particularly on the lower part. The extrudate that was printed with higher overflow ratio tends to deform inherently from the nozzle shape as a result of slump phenomenon as indicated on the lower part.

Fig. 16: The predicted extrudate geometry for a fixed rectangular nozzle with the localized overflow ratio ranging from 1.05 to 1.40

Subsequently, different nozzle shapes were analyzed together with varying overflow ratio. Five different nozzle shapes were considered and two overflow ratio values, i.e. at 1.1 and 1.4, were selected to analyze the nozzle shape influence.

Fig. 17 shows the results of the extrudate geometry prediction with the varying parameters. The nozzle shape has a more significant influence to the extrudate geometry when the overflow ratio is at 1.1. However, when the overflow ratio is set higher, it can be seen that the overflowing effect becomes more significant. This implies that at high overflow ratio the nozzle shape geometry would be less effective in playing its role. In other words, controlling

nozzle shape to achieve a designated extrudate geometry is only feasible when the overflow ratio is close to, but not less than, one.

Fig. 17: The predicted extrudate geometry for (a) 5 different nozzles with the localized overflow ratio at (b) 1.1 and (c) 1.4

4.5. Applying the trained model for improving printing quality

A database containing ten million random nozzle shapes and the corresponding predicted extrudate cross-sectional shapes was generated and used to find nozzle shapes for designated extrudate cross-sectional shapes. As the first case study, we considered printing a 15-degree inclined wall as illustrated in Fig. 18(a). The interior part of the inclined wall has infilled extrudate to support the inclined structure. The unique feature of the wall requires a specific extrudate shape as shown in Fig. 18(b) that was analyzed from the CAD model of the designated wall. Using the generated database, the corresponding nozzle geometry was obtained as indicated in Fig. 18(c), where subsequently the analyzed nozzle was fabricated and used for printing the wall.

As a benchmark, a common rectangular-like nozzle shape was used to print such targeted wall and the result is shown in Fig. 19(a). It can be easily observed that the wall printed with the

predicted nozzle shape, as shown in the Fig. 19(b), exhibits better quality than the prior. Quantitatively, Fig. 19(c) and (d) illustrate the roughness profiles of the printed walls for the latter and prior cases, respectively, where the arithmetic averaged roughness (R_a) of the wall printed with the common rectangular is 1.178mm and that with the model-based nozzle is 0.745mm.

Fig. 18: (a) The CAD model for printing inclined wall and the desired extrudate near the outer surface (b) the target extrudate cross-sectional shape (c) the nozzle predicted by the database to print the target extrudate cross-sectional shape

Fig. 19: (a) Visible staircase effect on the inclined wall printed using a rectangular nozzle,
 (b) reduced staircase effect on a printed wall using the predicted nozzle, surface roughness
 profile for walls printed using (c) rectangular nozzle and (d) predicted nozzle

In the second case, a simple vertical wall will be evaluated to see if the wall property, in terms of the roughness, can be improved using the proposed approach. The same database that was used in the previous study was also employed to determine the most optimal nozzle shape to

print such a wall. Similar as in the previous test, as a benchmark the same designated wall was also printed using a common rectangular nozzle. Fig. 20(a) and (b) illustrate the results of vertical walls printed using the rectangular nozzle and the analytic nozzle, respectively. The figures show that steps and gaps on the side of the wall are significantly reduced on the wall printed with the analytic nozzle compared to that printed by the rectangular nozzle. The improved surface profiles to conform the qualitative observation are shown in Fig. 20(c) and (d) correspondingly. The arithmetic averaged roughness (R_a) are 0.382mm and 0.695mm for the prior and latter cases, respectively. The result from the proposed approach exhibits a comparable surface finish quality to that obtained through experimental iteration approach as presented by Lao et al. [52]. However, in the current proposed approach the analysis requires much less processing time and it has been shown from the previous test that the approach also capable of printing a broader range of extrudate formation.

Fig. 20: The surface finish enhancement of a vertical wall printing comparing between (a) rectangular nozzle and (b) predicted nozzle printing (c) shape of the predicted nozzle and the surface roughness profile for (d) rectangular nozzle (e) ANN predicted nozzle

As the final case, a more complex part with a dynamic-curvature surface was also considered. The targeted wall comprises a curvy surface, where consequently the required target extrudate shape is not identical in every layer. For the sake of simplicity, in this validation test one specific nozzle will be used to print three layers of extrudate. Every 3 layers, the printing

process would be paused, and the nozzle would be replaced by another analyzed nozzle appropriated for the next 3 layers.

As a benchmark, similar as in the previous tests, the curvy wall was also printed using a common rectangular nozzle. The parts, subsequently, were sliced and analyzed. The cross-section of the part printed with rectangular and that printed with the analytical nozzle are shown in Fig. 21(a) and (b), respectively, where for quantitative measure, the roughness profiles of the corresponding samples are shown in Fig. 21(c) and (d). The arithmetic averaged surface roughness (R_a) of the part printed with rectangular nozzle was 1.170 mm, while that with the analytic nozzles is 0.788mm. The results show that the proposed model-based nozzle design allows for improving the printed wall surface quality by adjusting the nozzle outlet shape. However, it is acknowledged that in the experiment, the nozzle-changing process that was carried out after three printed extrudate layer is impractical. Moreover, the start-stop practice in the printing process might cause instability in the overflow ratio. Therefore, a smart-active nozzle with a capability to vary its geometry will facilitate to control the extrudate geometry, especially on dynamic-curvature wall printing. The mechanism is currently under development at SC3DP/NTU facility and the results will be communicated in the subsequent publication.

Fig. 21: The surface curvature of concave wall printing using: (a) rectangular nozzle and (b) analytical nozzle. Surface roughness profiles for concave walls using: (c) rectangular nozzle and (d) analytic nozzle.

5. Conclusion

In this paper, we have demonstrated a predictive modeling-based approach to directly control the geometry of 3DCP extrudate with different shapes of nozzle. Thirteen different nozzle shapes were predetermined and fabricated, where subsequently used to produce some extrudates. The cross-sectional shapes of the nozzles together with the corresponding extrudate geometry images were analyzed with the help from MATLAB. A predictive model was, therefore, developed to correlate between the nozzle shape and the extrudate shape counterpart using ANN. Upon the accomplishment of the model development, a nozzle-extrudate database was formed to allow for analyzing the optimal nozzle shape for a specific target extrude shapes. The results show that the proposed approach offers the improvement of the surface quality on three structures with different curvature by adapting the nozzle geometry according to the corresponding targeted extrudate shape.

Comparing with the benchmarking rectangular-shaped nozzles, this approach showed obvious improvement to the surface finish quality. More importantly, the proposed approach showed strong flexibility to facilitate surface finish improvement for different types of printing structure. This approach has a theoretical potential to improve surface finish quality for any kind of 3D printable structures, because it directly applies shape control to the smallest engineering component of 3DCP, the extrudate, and make it adopt to the structure's curvature. At the current stage of 3DCP where the surface finish quality is too rough to overlook but compromising printing speed to trade surface finish quality is obviously impractical, the proposed approach could be an innovative solution to improve quality control in 3DCP technology.

Hypothetically, this method might be useful for other material-extrusion 3D printing because the deposition process takes the similar principle. Although changing the nozzle shape in a different process conditions can be challenging, the finding in this study still offers an idea to improve the printing quality by controlling the extrudate formation in other extrusion-based 3D printing.

Our primary future plan is to extend the concept into in-situ printing. The major obstacle between the concept and the application is the lack of a nozzle which has a real-time controllable outlet geometry. A variable-geometry nozzle prototype is designed to have a variable-geometry outlet and is being tested in SC3DP. In the meantime, we will continue improving the machine learning model to include more process parameters of 3DCP in the future.

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