# **Pore in Concrete-Group8**

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# **CEE 498 Project: Characterization of Porosity in Cement Paste Matrix**

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#### **Abstract**

This research investigates applicability of image-based analysis to quantify and classify porosities in grayscale scanning electron microscopy (SEM) images, made from polished thin section of hydrated cement beams. Within the past decades, mercury intrusion porosimeter (MIP) technique has been used to measure pore volume fraction in cement-based matrices. However, MIP method was found to overestimate porosity as it is incapable of quantifying disconnected pores. Therefore, it is of interest to determine whether image analysis coupled with Artificial Neural Network (ANN) or Convolutional Neural Network (CNN) could characterize porosity. Accordingly, images pre-analyzed by ImageJ commercial software are used to calibrate the python code. The calibrated model was used for Exploratory Data Analysis (EDA) for feature engineering. The extracted features, which are likely to be predictive of porosity, are used to train the employed machine learning models. Results of the present study revealed the applicability of ANN for estimating porosity based on physical properties of pores and chemistry of hydrates. Also, CNN is found to be an efficient way of classifying SEM images having different pore volume fraction. The present research has the potential to be used in future to predict the remaining service life and the physicochemical properties of the cement matrix.

#### **Keywords:**

Scanning Electron Microscopy (SEM), Mercury Intrusion Porosimeter (MIP), Artificial Neural Network (ANN), Convolutional Neural Network (CNN), Exploratory Data Analysis (EDA), porosity

# Introduction

Durability of concrete structures against gradual ingress of deleterious liquids is mainly controlled by porosity and pore structure of cement paste matrix [1]. Pore structure is mainly divided into two main categories: capillary and gel pores and they range from few millimeters into few nano-meters having 70-90% of total porosity in the nano scale. There are multiple factors that affect general properties of capillary pore structure in concrete, which include curing regimes, cementitious materials contents, and water-to-cementitious materials ratios [1-2]. Therefore, it is necessary to precisely measure and characterize pore structure in concrete to determine the optimum concrete curing conditions and mix proportions.

Over the past few decades, mercury intrusion porosimeter (MIP) test has been used to measure porosity and pore size distribution in cement-based composites. In this method, using relatively high pressure, mercury is injected into the pore spaces of the matrix to determine porosity and its structure. MIP test, with an ability to measure pore sizes in the range of 0.006–500 µm, is typically performed on a small oven-dried cement-composite specimen and mercury is gradually applied on the desired surface [1]. However, it has been reported that, cement matrix surface tension as well as mercury contact angle with cement pore wall affects the accuracy of MIP measurements [3]. Moreover, MIP needs speciemn preparation; it is hard to conduct; and it is deemed a destructive test in such it damages weak microstructure due to the applied high pressure.

To address the uncertainty of MIP results, image analysis method is recently developed to directly measure paste matrix porosity. Backscattered scanning electron microscopy (SEM) images of polished impregnated epoxy concrete surface is captured and analyzed using ImageJ commercial software [1]. To go further, ImageJ software quantifies the total area of pores using a grayscale thresholded image. However, this commercial software solely provides total porosity of the matrix and lacks the ability to characterize porosity [1]. In addition, comparing the total porosity of paste matrices measured by MIP method with that measured by ImageJ revealed that porosity is underestimated in the former technique. In fact, in contrary to MIP, Image analysis is capable of measuring both connected and disconnected capillary pores, and hence gives a more realistic picture of the paste matrix pore system [1]. Also, SEM technique is easy to conduct since it does not need and specimen preparation, but costs a lot of money.

As a result, it is required to develop an image analysis-based technique to not only determine total porosity, but also characterize the pore structure, such as shape, size, and angularity of the pore system. For this reason, robust codes are written in python to read and analyze greyscale thresholded 200 SEM images. The present analysis is calibrated by matching average porosity found by python-based image analysis with that of ImageJ software. The calibrated model is then used to read images to find pore size distribution of the matrix. In the next step, chemistry of hydrates and angularity of pores are estimated to be used as features for the employed machine learning algorithms. Results of the present analysis revealed that ANN is a robust technique being capable of correlating pore volume fraction with angularity of pores, as well as chemistry of hydrates. In addition, porosities are classified into different categories using an optimized CNN. The relatively low Root Mean Squared Error (RSME) values of the two machine learning techniques, i.e. ANN and CNN, proposes the robustness of the present methodology over MIP for characterizing porosity in cement paste matrix.

# **Methods:**

## **Exploratory Data Analysis**

Exploratory data analysis (EDA) is an important step conducted on any data analysis project for identification, characterization, and quantifiaction of different features. In this project, our input data consists of two columns, images (IDs) and their corresponding porosity, which were determined by ImageJ commercial software. Fig 1 shows porosities of five random images for each batch, with porosities variable from 0 to 100 percent.

#### Batch1

	batch1_image_id	porosity(%)
0	batch1:image_1_1	37.022000
1	batch1:image_1_2	18.738000
2	batch1:image_1_3	15.658000
3	batch1:image_1_4	18.941000
4	batch1:image_1_5	0.397000

#### Batch2

	batch2_image_id	porosity(%)
0	batch2:image_1_1	18.656000
1	batch2:image_1_2	23.989000
2	batch2:image_1_3	16.622000
3	batch2:image_1_4	17.122000
4	batch2:image_1_5	20.068000

Figure 1: importing tabular data for EDA

The data set has two batches and each batch has 100 images, which will be used for porosity characterization. In the next step, images are read to facilitate understanding of the general characterestics of pore system. The first three images chosen from batch1 are shown in Fig 2:

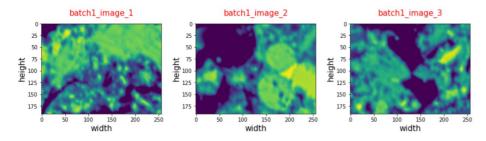


Figure 2: importing first three images from batch1

As shown in Fig 2, images were shown in Viridis color system. However, there are two problems associate with the Viridis color system used for reading images. Firstly, there is a significant variation of color for thresholds ranging from 0 to 10, hence porosity quantification may subject to instability. Secondly, identification and quantification of cement hydration products has been done in Greyscale color system [1]. Consequently, it is required to convert Viridis to Greyscale color system to enahnce accuracy of EDA. Fig 3 provides a comparison of these two different color systems

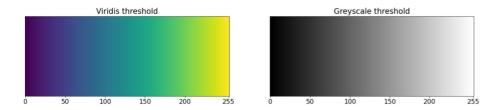


Figure 3: comparison of Viridis vs. Greyscale color systems for reading images in python

As previously mentioned, the color system of images had to be converted to Greyscale to faciliate chemical analysis of hydartes, and ease quantification of porosity in cement paste matrix. In Fig 4, it is shown that pixels having darker luminance belong to capillary pores, intermediate thresholds belong to hydrated products, while higher thresholds belongs to cement hydarted products.

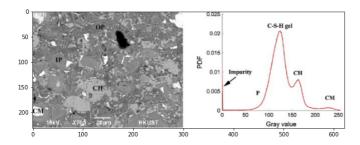


Figure 4: identifiaction and quantification of different phases using greyscale SEM images

As a result, Fig 5 shows a converted version of Fig 1 transformed from Viridis to Greyscale, which will be used for EDA.

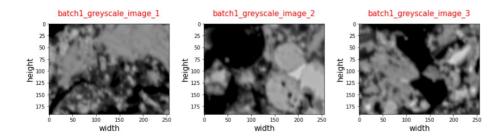


Figure 5: transformation of input images from Viridis to Greyscale

#### **Model Caliberation**

To quntify porosity and other characterestics of images, including chemistry and angularity of pores, it is a required task to caliberate the model. The input grayscale images are all having 256\*196 pixels with grayscale thresholds ranging from 0 to 255; dark pixels represent pores, while pixels with higher thershold values represent cement hydrated or anhydrous products. To quantify pore volume fraction, different thresholds correspond to pores are chosen to determine the impact of threshold limit on the averge porosity (see Fig 6). Fig 6 illuminates the maximum thresholds for both batches (i.e. 14 and 9 for batches 1 and 2, respectively), which avoids overestimation of porosity in both batches. Almost 400 million pixels were analyzed to generate this figure.

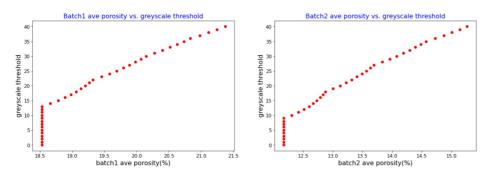


Figure 6: quantification of average porosity vs. threshold limits

Figs 7 and 8 represent the important role of assigning a correct threshold value for characterizing porosity. In other words, increasing the luminance (threshold) of images from a certain limit (i.e. i.e. 14 and 9 for batches 1 and 2, respectively) will result in the inclusion of dark hydration products (i.e. precialse or luminance), which has to be avoide.

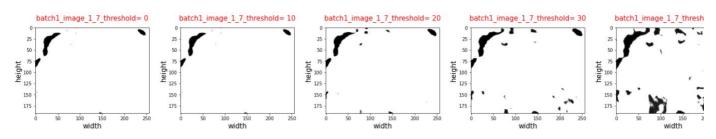


Figure 7: dependence of batch1 porosity on the assigned luminance

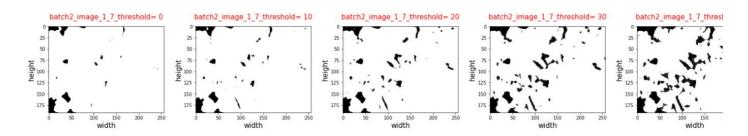


Figure 8: dependence of batch1 porosity on the assigned luminance

Therefore, luminance of images should be assigned carefully to realistically estimate porosity with minimum error. Fig 9 further illuminates dependence of image analysis on the assigned threshold. In this figure, the exact porosities of images found from ImageJ software are comapred with those estimated using EDA for both two batches. This comparison reveals that as long as the luminance is limited to 10, calculated porosities remain stable and accurate, while exceeding this limits results in over estimatetion of porosites.

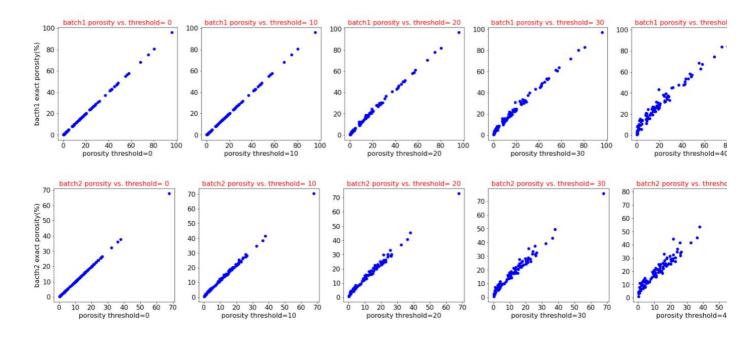


Figure 9: matching estimated porosities with exact porosities for different threshold limits

Considering Fig 9, the threshold limit = 0 is finally chosen to accurately estimate the porosity of images.

## **Chemical Analysis**

As previously mentioned, greyscale SEM images are required to be considered for chemical analysis. The following thresholds intervals are defined for each image to characterize different phases:

- Capillary Pores: 0 < threshold < 1
- Magnesium/ Sulphur: 10 < threshold < 70
- Calcium Silicate Hydrates (C-S-H): 70 < threshold < 140
- Calcium Hydroxide (C-H): 140 < threshold < 180
- Unknown (Anhydrous/ Aluminum): 180 < threshold < 255

To determine the robustness of image-based chemical analysis, a random image from batch1 is selected and characterized in Fig 10.

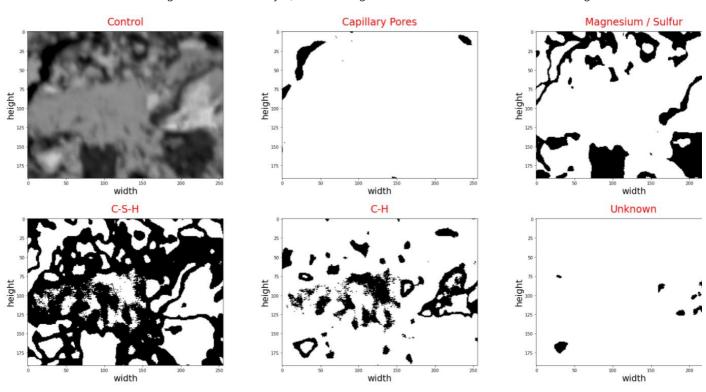


Figure 10: chemical analysis of greyscale SEM images

In the next step, the shape of capillary pores is characterized using a terminology called angularity. For this purpose, a dimensionless formula is defined to calculate angularity based on the total perimeter and area of capillary pores of each figure:

$$Angularity = log \frac{Perimeter^2}{4\pi Area}$$

As shown in the Fig 11, for capillary pores having similar area, the perimeter increases with angularity. In other words, pores having similar perimeter but less angularity have larger areas.

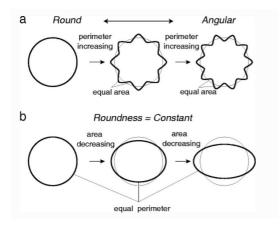


Figure 11: comparing round vs angular shapes

Accordingly, it is required to calculate area and perimeter of capillary pores in each figure. Based on trial and error attempts, the threshold interval for calculating area of pores is 0 < threshold < 1, while to estimate perimeter, the interval is modified to 1 < threshold < 30. Also, incorporating higher threshold limits (i.e. 30 < threshold < 60) would include hydrates having relatively darker luminance, e.g. magnesium or brucite, that may result in overestimation of porosity. Fig 12 shows estimation of total area as well as total porosity, as a function of luminance interval, for estimating angularity of each image.

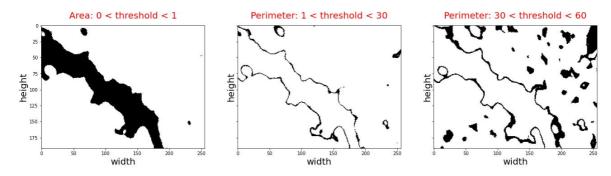


Figure 12: estimating parameters of angularity

## **Modeling**

The ANN models shown below explain how cement chemistry (model I) together with a combination of cement chemistry and pore physical shape (model II) could be used to estimate porosities, i.e. output, of testing batch 3 (Fig 13).

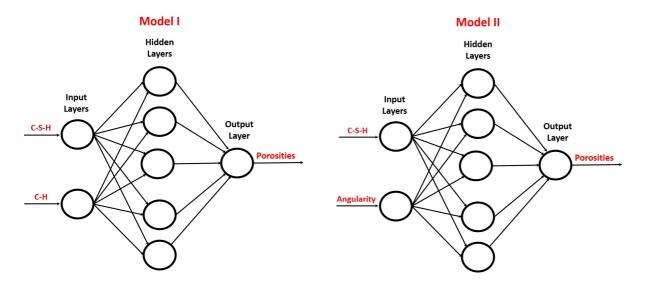


Figure 13: ANN models used for estimating porosities

The first step for doing ANN is to determine the type of variables used for training the datasets. As shown in Fig 14, the variables shown are all in float 64 type. However, only float32 datatype works well for tensor flow, and the variables are hence converted to this datatype.

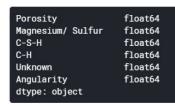


Figure 14: Representing the type of input variables

The structure of employed ANN model consists of layers having different complexities, which are placed sequentially. As well, 1024 intermediate nodes are generated by matrix multiplications using ReLU rectifier to facilitate prediction of the nonlinear model, see Fig 15. To control the speed and quality of learning process, the value of other hyperparameters including, learning rate, epochs, and batch size are set to be 0.0001, 300, and 50, respectively.

```
def create_model(learning_rate, feature_layer):
    model=tf.keras.Sequential()
    model.add(feature_layer)

model.add(ff.keras.layers.Dense(units=1024, activation ="relu",kernel_regularizer = tf.keras.regularizers.11_12(11=0.005, 12=0.005)))
    model.add(tf.keras.layers.Dense(units=1024, activation ="relu",kernel_regularizer = tf.keras.regularizers.11_12(11=0.005, 12=0.005)))
    model.add(tf.keras.layers.Dense(units=10))

model.add(tf.keras.layers.Dense(units=1))
model.compile(optimizer=tf.keras.optimizers.Adam(lr=learning_rate), loss="mean_squared_error", metrics=[tf.keras.metrics.MeanSquaredError()])
return model
```

Figure 15: Creating ANN model to estimate porosities

A model has been built using Convolutional Neural Network (CNN) approach. Having the images from the training set coincided with their labels (porosity values) as the input of the model. This model will be freezed while fetching and processing a previous model performed on a very big data (images). The usual image data set "imagenet" is used as a preprocessed model to let the model train in a complex way to understand and identify images. Due to having a very limited number of images, we had to divide porosity into categories in order to make it easier to the model to predict for a limited number of outputs (labels). This division was done by some of the team members as a way of variety in this project. However, in any real case study, specifing categories will be needed to make it more reasonable to predict physiochemical properties such as freezing and thawing since freezing and thawing behavior for example is changing discretely e.g. very poor, poor, acceptable, good, very good.

Image augmentation is pretty important in image processing. As we deal with pixels values and shapes, we focused on image flipping and sizing augmentation rather than color augmentation since we deal with grayscale images and pixels values.

Regarding the model, it was not different from what was given in the class. Manipulation of hyperparameters was critical in order to achieve a satisfactory accuracy. Fig 16 shows the model and Fig 17 shows the used hyperparameters in the CNN model. The used epochs is 80, and learning rate is 5.0 e-5.

```
height, width = 192, 256
base_model = keras.applications.Xception(
    weights="imagenet",
    input_shape=(height, width, 3),
    include_top=False,
base_model.trainable = True
inputs = keras.Input(shape=(height, width, 3))
from tensorflow.keras.optimizers import RMSprop
norm_layer = keras.layers.experimental.preprocessing.Normalization()
mean = np.array([127.5] * 3)
var = mean ** 2
x = norm_layer(inputs)
norm_layer.set_weights([mean, var])
x = base_model(x, training=False)
x = keras.layers.GlobalAveragePooling2D()(x)
x = keras.layers.Dropout(0.1)(x)
num_outputs = 4
\verb"outputs" = keras. \underline{layers.Dense}(\texttt{num\_outputs}, \ \texttt{activation="softmax"})(\texttt{x})
model = keras.Model(inputs, outputs)
model.summary()
```

#### Figure 16: the CNN model algorithm

```
learning_rate = 5.0e-5

model.compile(
    optimizer=keras.optimizers.Adam(learning_rate=learning_rate),
    loss= tf.keras.losses.SparseCategoricalCrossentropy(),
    metrics=[tf.keras.metrics.SparseCategoricalAccuracy()],
)

epochs = 80
history = model.fit(ds_train2, epochs=epochs, validation_data=ds_test2)
```

Figure 17: hyperparameters for CNN model

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