Supplementary information to

Elucidating the Auxetic Behavior of Cementitious Cellular Composites Using Finite Element Analysis and Interpretable Machine Learning

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A. Mesh convergence study

In order to show that the effective properties obtained using finite element analysis are converged, a mesh-convergence study for the representative unit cell of mortar mesostructure is carried out. Figure S1 shows the results of the mesh-convergence study. The goal is, to find the number of elements that satisfies a sufficient grade of accuracy and simultaneously optimizes the time feasibility. A mesh beyond 12491 4-node bilinear, reduced integration elements (CPE4R in ABAQUS), yields a converged solution. Thus, a total of 12491 elements are implemented. Thereby, the chosen element number of elements adequately capturing the effective Poisson's ratio of the unit cell. The chosen elements invoke a trade-off between computational expense and prediction efficiency.

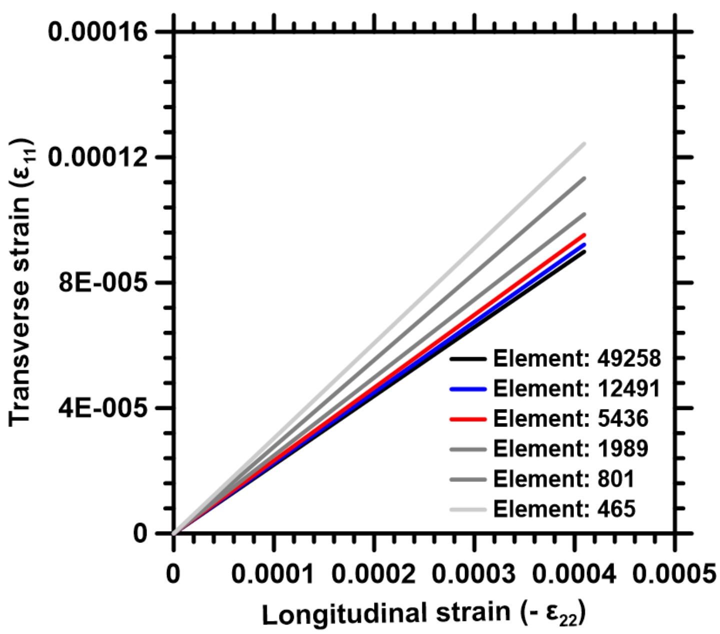

Figure S1. Mesh convergence

B. Geometries

Figure S2 demonstrates the model geometry with various aspect ratios for a constant length of the major axis, and the same number of voids along the X-axis and Y-axis. The subfigure in Figure 2(a) indicates the minor axis and the major axis for one void. The major axis is always the longer axis. The minor axis is calculated by the length of the major axis divided by the aspect ratio. It can be seen that with a constant number of voids and length of the major axis, the porosity decreases with an increasing aspect ratio.

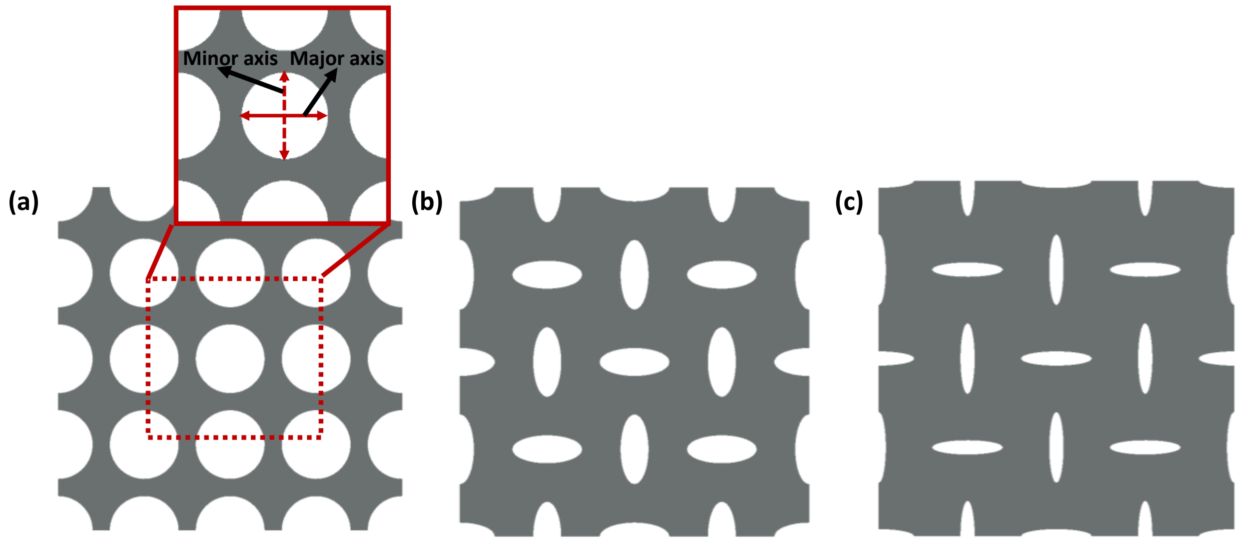

Figure S2. Model geometry with 6 mm length of the major axis for aspect ratio of (a) 1, (b) 2.5, (c) 4. The number of voids in x-direction and y-direction is identical and equals 4.

Figure S3 depicts the model geometry with variations in the number of voids along the X-axis and Y-axis for a constant aspect ratio and length of the major axis.

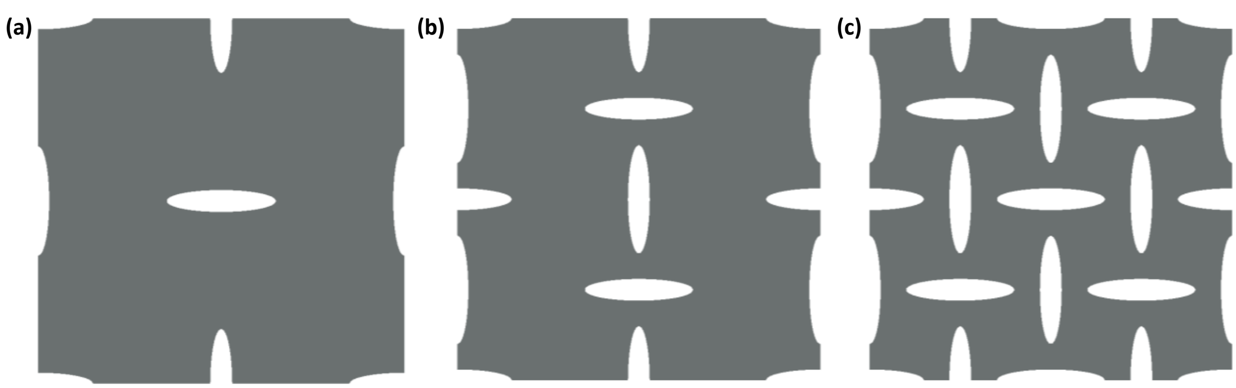

Figure S3. Model geometry with number of voids (a) N_x = 2 and N_y = 2, (b) N_x = 2 and N_y = 4, (c) N_x =4 and N_y = 4 for a constant aspect ratio of 5 and length of major axis = 15 mm. The number of voids in x-direction and y-direction is denoted as N_x and N_y, respectively.

In this case, the porosity increases with the increase in the number of voids along the two axes. Figure S4 illustrates the change in the model geometry when the length of the major axis increases for a constant aspect ratio and the number of voids. The porosity increases with the increasing length of the major axis.

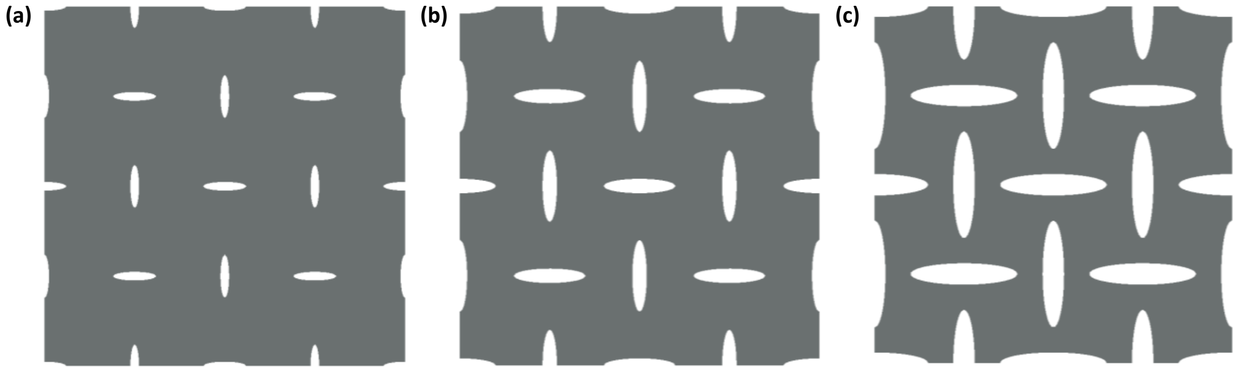

Figure S4. Model geometry for the major axis length of (a) 6 mm, (b) 10 mm and (c) 15 mm with a constant aspect ratio of 5 and number of voids in x-direction and y-direction is identical and equals to 4.

C. OPTIMIZED NEURAL NETWORK

The optimized neural network that relates the input arguments (volume fraction, number of voids along X-axis, number of voids along Y-axis, aspect ratio, and major axis length) can be written as:

$$Y = \boldsymbol{b}^{(3)} + \boldsymbol{w}^{(3)} \times f_{ReLu}\left(\boldsymbol{b}^{(2)} + \boldsymbol{w}^{(2)} \times f_{ReLu}\left(\boldsymbol{b}^{(1)} + \boldsymbol{w}^{(1)}\boldsymbol{X}\right)\right)$$

$\boldsymbol{w}^{(1)}$ = [0.91322595, 0.24670811, 0.05722396, 0.76339287, -0.06510681,
0.61609274, 0.55018574, 0.3979613 , 0.40044287, -0.30405957,
0.6439572 , 0.2966507 , -2.7511754 , -2.6358175 ;
0.56605107, -0.63538396, 0.06659086, -0.5802128 , 0.23002961,
-0.08426097, -0.12857582, 0.4197393 , -0.0996479 , -0.64983803,
0.41779512, 0.21776183, -0.3014933 , -0.45530313;
-0.46967733, 0.00705126, 0.23710203, 0.2943382 , -0.516587 ,
-0.8245896 , 0.16972306, -0.50078547, -0.62435615, -0.2861971 ,
-0.24208695, 0.73075706, 1.2354326 , 0.96411;
0.29110438, 0.30321816, -0.1287605 , 0.6631742 , 0.4108077 ,
0.20697476, 0.10090452, -0.25769213, 0.555713 , -0.40484363,
-0.14802422, 0.04289406, -0.98477906, -0.90970623;
0.226125 , 0.16086687, 0.03054334, -0.5343891 , -0.12141306,
-0.21728037, -1.2440838 , 0.00921982, -0.9716563 , 0.06647905,
0.06081539, 0.66588235, -0.22415428, -0.38810757]

$\boldsymbol{b}^{(1)}$ = [-0.05000221, -0.36172467, 0.06094412, 0.138616 , 0.21590742,
-0.22535689, -0.38624004, -0.16470669, 0.10655642, -0.6504957 ,

-0.39687607, -0.39622706, 0.08490311, 0.03725716]

$\boldsymbol{w}^{(2)}$ = [6.56180978e-01, -8.02664220e-01, 4.40794408e-01,
4.07692790e-02, 1.96262598e-01, -8.32270324e-01,
-6.06589854e-01, -2.27561712e-01, 2.48609394e-01,
-1.61018622e+00, 6.00405693e-01, 1.12511724e-01,
3.66302907e-01, 1.93363279e-01;
9.60397899e-01, 3.65349442e-01, 4.11751494e-02,
1.45602062e-01, 3.64076525e-01, 4.27577347e-01,
5.98402500e-01, -4.23993826e-01, -1.07417062e-01,
-8.82345438e-01, -3.80377889e-01, -2.73667037e-01,
-6.58972442e-01, -4.29031670e-01;
3.04709941e-01, 1.48785254e-03, -1.79837739e+00,
-5.56240305e-02, 5.12268007e-01, 9.97751117e-01,
-3.97541255e-01, -1.72034368e-01, -9.98617411e-02,
-9.85821187e-01, 2.53557712e-01, -6.62896335e-01,
4.56911400e-02, -2.84199804e-01;
-3.84369463e-01, 4.00952369e-01, 1.66070275e-02,
8.66386294e-03, -7.39777908e-02, -2.11691801e-02,
-2.41620392e-01, 4.17011410e-01, 1.16409898e-01,
-1.78951815e-01, 1.39636472e-01, -3.21765989e-01,
-2.97177982e+00, 1.17783773e+00;
-1.03217892e-01, -2.07332477e-01, -9.84980106e-01,
4.76857275e-01, -8.81835759e-01, 9.62375164e-01,
-4.79249563e-03, 1.00863293e-01, 8.30341950e-02,
4.57094371e-01, -6.47272587e-01, -5.43985562e-03,
2.12295484e-02, -3.91770639e-02;
-8.79772758e+00, 1.13930798e+00, -1.19930327e+00,
-3.56705040e-01, -3.74450028e-01, -5.42134464e-01,
5.06798148e-01, -3.81902307e-01, -1.72258615e-01,
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-2.65401136e-02, -1.04061306e-01;
3.37617069e-01, -1.48295537e-01, 6.46392465e-01,
-3.62023376e-02, -7.57977545e-01, 1.04817176e+00,
2.06125990e-01, 4.42961216e-01, -1.29938558e-01,
-5.09385943e-01, -6.43154025e-01, 4.54638511e-01,
-2.93732166e-01, -2.34493211e-01;
-4.88685936e-01, 2.48331487e-01, -1.39851332e+00,
1.34743199e-01, -5.67143746e-02, -6.26967716e+00,
4.06053543e-01, 8.38739276e-01, 3.24373960e-01,
-1.11036301e-02, -8.30311835e-01, 6.83155179e-01,
-1.30128682e+00, 5.57035625e-01;
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-2.32210651e-01, -1.19758986e-01, 1.82763577e-01,
4.77200061e-01, -6.29222929e-01, -3.95190150e-01,
-4.52442020e-01, 7.58755624e-01, 3.83921146e-01,
2.71226943e-01, 6.56589031e-01;
-5.63719809e-01, 6.07276380e-01, -4.07453895e-01,

1.91210598e-01, 3.14055741e-01, 3.87932599e-01,
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-5.80197573e-01, -4.70285863e-01, 5.05804658e-01,
3.26354861e-01, 2.48162940e-01;
-7.70203173e-01, 4.03975427e-01, 7.21043646e-01,
3.31595898e-01, 1.82833448e-01, -3.61672378e+00,
5.74926324e-02, -4.81865585e-01, 1.41238300e-02,
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1.79331571e-01, -7.58141816e-01, -2.32278132e+00,
9.80619192e-01, -3.75706553e-01, -8.38524878e-01,
5.75271854e-03, 3.27003866e-01, 6.96828127e-01,
-7.69516850e+00, -3.65479916e-01, 1.40762497e-02,
1.68246031e-01, -6.10290356e-02;
-1.00106764e+00, -1.96918130e-01, 6.55199289e-01,
-1.31288328e+01, -1.60066068e+00, 7.37734973e-01,
1.51381373e+00, -1.49962708e-01, -1.79832208e+00,
-5.22246301e-01, 7.56698728e-01, 1.56572974e+00,
-5.44374943e-01, -1.63930774e-01;
1.07340693e+00, 2.29305737e-02, -7.73491502e-01,
-2.41605401e+00, 1.37566948e+00, -8.58007967e-01,
-1.66511953e+00, 6.07257068e-01, 1.75533068e+00,
5.96098542e-01, -1.03332627e+00, -1.71470273e+00,
-3.93675625e-01, 2.28641316e-01]

$\boldsymbol{b}^{(2)}$ = [-0.09684628, 0.8852983, 0.21008632, -0.2101158 , 0.18566458,
-0.75970465, -0.16613844, 0.17431176, 0.01891873, 0.3260775 ,
0.5187125, -0.12627897, -0.31615737, 0.00494562]

$\boldsymbol{w}^{(3)}$ = [0.16564372,
0.19792055,
0.1018835,
0.2835567,
0.11930594,
0.15443729,
-0.4498774,
0.11316536,
-0.30917174,
0.07340249,
-0.14367038,
0.24108705,
1.3914852,
-0.11234241]

$\boldsymbol{b}^{(3)}$ = -0.05904523;

The input arguments followed a standardized scaling written as:

$$\boldsymbol{X} = \left\{\frac{x_i - \mu_i}{\sigma_i}\right\}, i = 1,2,3,4,5$$

μ = [0.1848771, 3.59646539, 4.71281296, 3.3365243, 11.36003494]

σ= [1.43354981e-02, 3.33053243, 3.28571212, 1.43645684, 4.38900177e+01]

where x is the input arguments, μ is the mean value, and σ standard deviation. f_{ReLu} is the sigmoid activation function written as:

$$f_{Relu}(x) = \max(0, x)$$