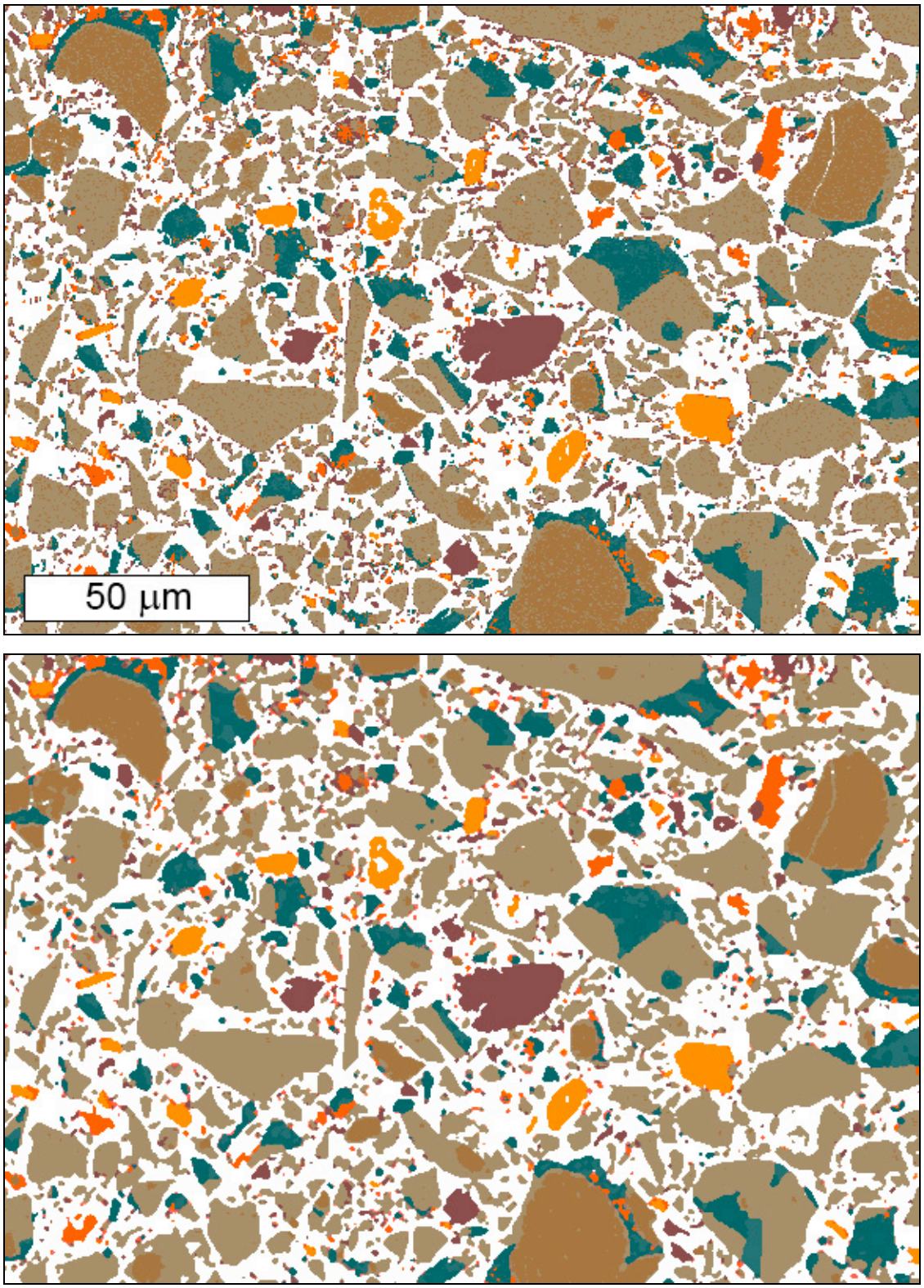

Figure 65: Classified image output (top) and after application of median filter to remove noise (bottom) to show major cement phases, color-coded as follows: brown = C_2S, tan = C_3S, dark blue green = C_4AF, light blue green = C_3A, orange = undifferentiated calcium sulfate phases, orange red = potassium sulfate, and dark red = interground limestone.

5.2.6.4 Determination of Cycle to Time Conversion Factor

When running the CEMHYD3D model, a conversion factor is required to translate the cycles employed by the model into real time. Since chemical shrinkage is one output of the CHMHYD3D model, the results of laboratory shrinkage tests were used to calibrate the model. During hydration, the volume of hydration products occupies less space than the volume of cement powder and water initially used. Shrinkage of this nature is termed chemical shrinkage. In order to measure the magnitude of this shrinkage, several laboratory test methods have been proposed. In this research, the method proposed by Tazawa et al. was adopted [1995] and is outlined in Figure 66.

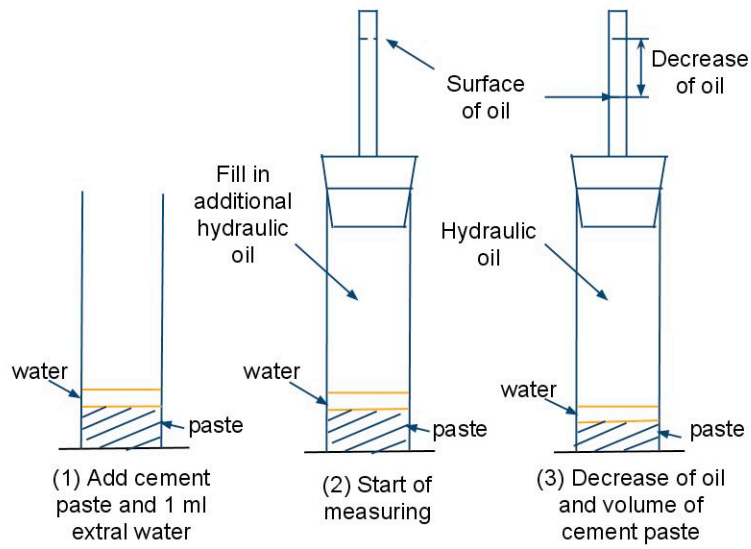

Figure 66: Depiction of chemical shrinkage experimental set-up, after Tazawa et al., [1995].

In the test, cement pastes were made using 10 g of cement and enough water to yield *w*/*cm* values of 0.45, 0.50, and 0.52. The pastes were mixed in the bottoms of 2.5 cm diameter glass tubes. An additional 1.0 ml water was added over the top of the cement paste in each tube, and the remainder of each tube was filled with hydraulic oil. The glass tubes were sealed with rubber stoppers encasing pipettes graduated in 0.01 ml increments. The tubes were kept in a 25 °C water bath along with a control sample containing only cement and oil to allow for corrections due to variation in temperature. As the cement pastes hydrated, the chemical shrinkage values were read from the oil levels in the pipettes.

To find an appropriate cycle to time conversion factor, several values were used as input for the CEMHYD3D disrealnew.c model, and the chemical shrinkage model outputs were plotted against the laboratory test results. By varying only the cycle to time conversion factor, it was not

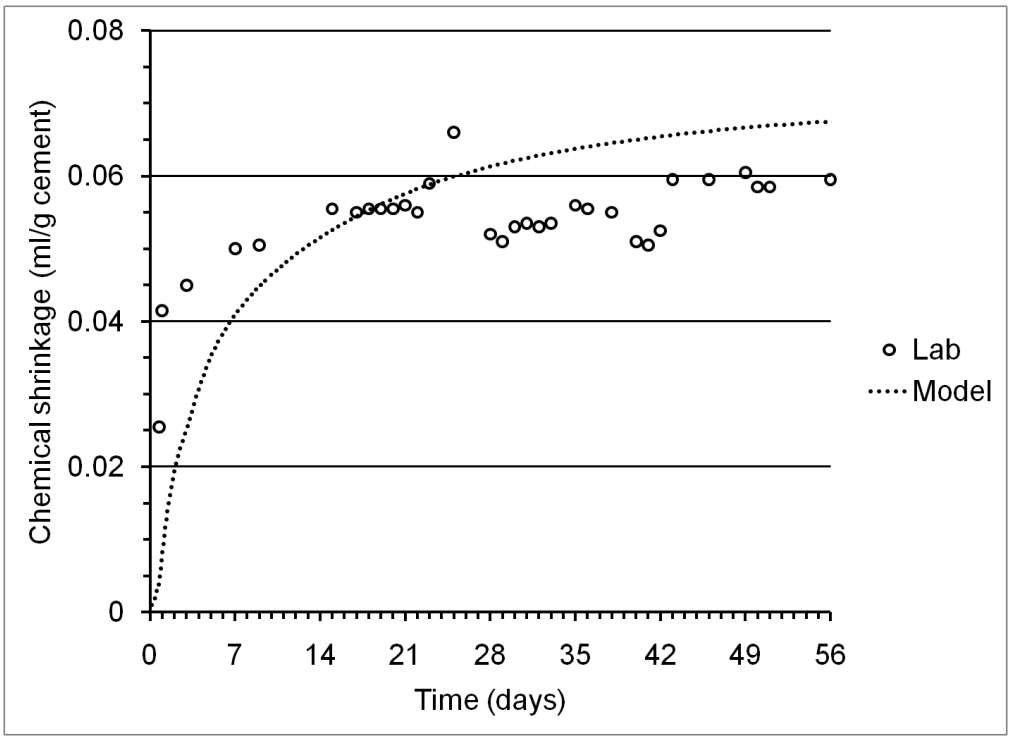

Figure 67: Laboratory and model chemical shrinkage data for 0.45 *w/cm* cement paste at cycle to time conversion factor of 0.00035.

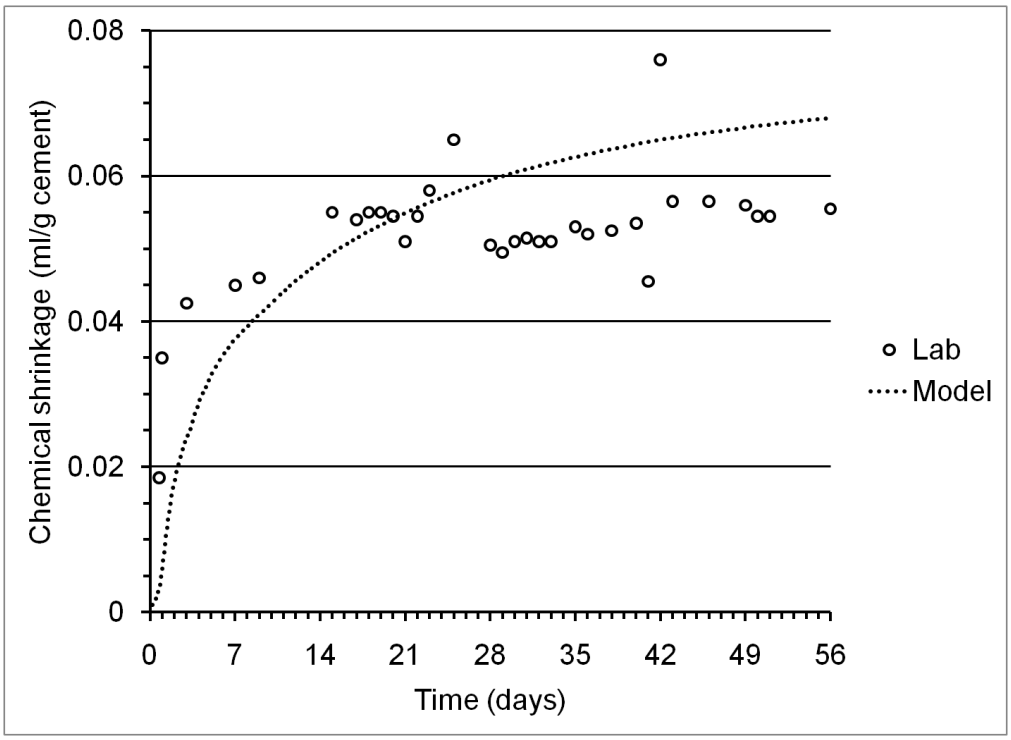

Figure 68: Laboratory and model chemical shrinkage data for 0.50 *w/cm* cement paste at cycle to time conversion factor of 0.00040.

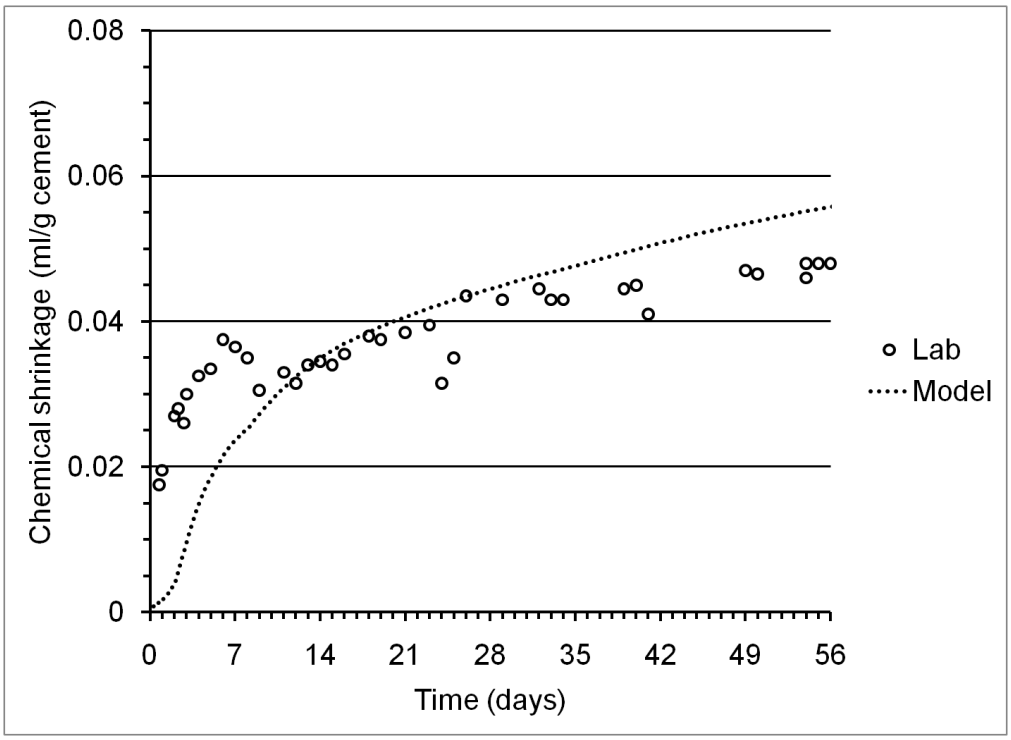

Figure 69: Laboratory and model chemical shrinkage data for 0.52 *w/cm* cement paste at cycle to time conversion factor of 0.00100.

possible to simultaneously achieve a good fit with both the short-term and long-term chemical shrinkage data. By trial and error, comparing model output to chemical shrinkage measured in the laboratory, cycle to time conversion factors of 0.00035, 0.00040 and 0.0010 were selected for the 0.45, 050, and 0.52 *w/cm* hydration models respectively in an effort to find a balance between the model deviations from the short-term and long-term laboratory data. The corresponding chemical shrinkage curves from the laboratory test and the model output are listed in Figures 67-69.

5.2.7 Execution of the Hydration Model

The CEMHYD3D program disrealnew.c was used to hydrate the 0.45, 050, and 0.52 *w/cm* systems. The bottom third of Figure 63 shows slices from the model output after 56 days of hydration. Figures 70 and 71 examine the development of the pore system over time for the hydration models. Figure 70 plots the total pore volume versus time, with the expected relationship of a decrease of porosity over time as the pore spaces fill with hydration products, and decreased porosity overall as the *w/cm* increases. Figure 71 plots the fraction of connected pores across the 0.1 mm wide cube. At time zero, the entire pore system is connected, but as time increases, larger fractions of the pore system become isolated, and the fraction of connected pores decreases. For the 0.45 *w/cm* scenario, the fraction of connected pores drops to zero after 40 days. The text of the input files used to run the hydration models are included in the Appendix.

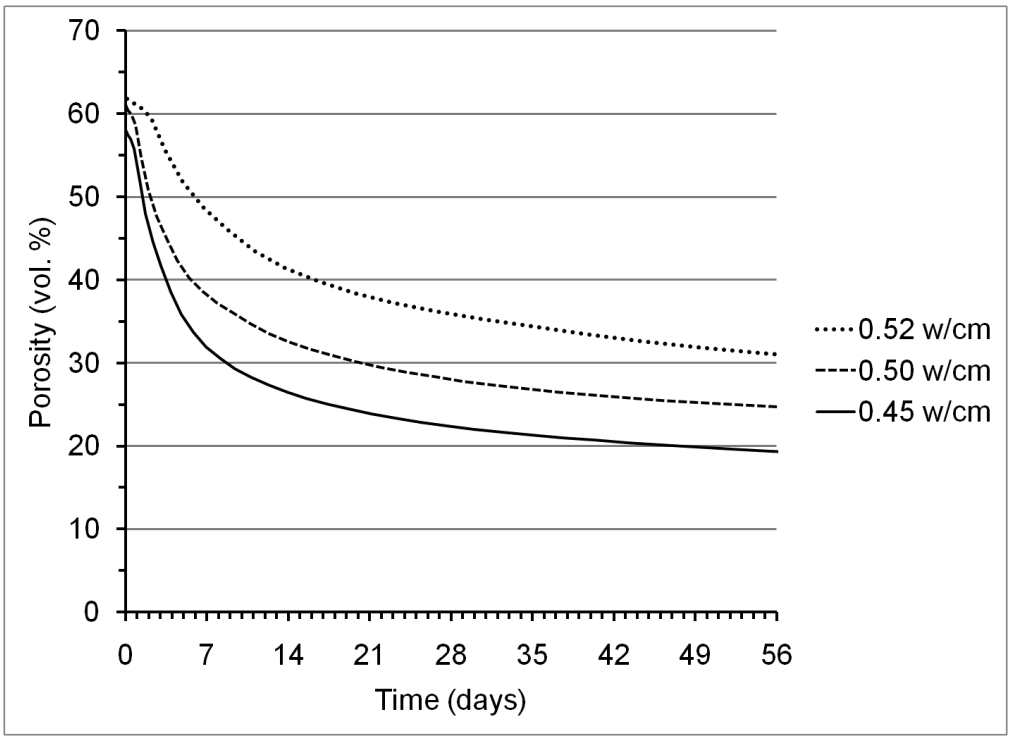

Figure 70: Total porosity versus time from the hydration models.

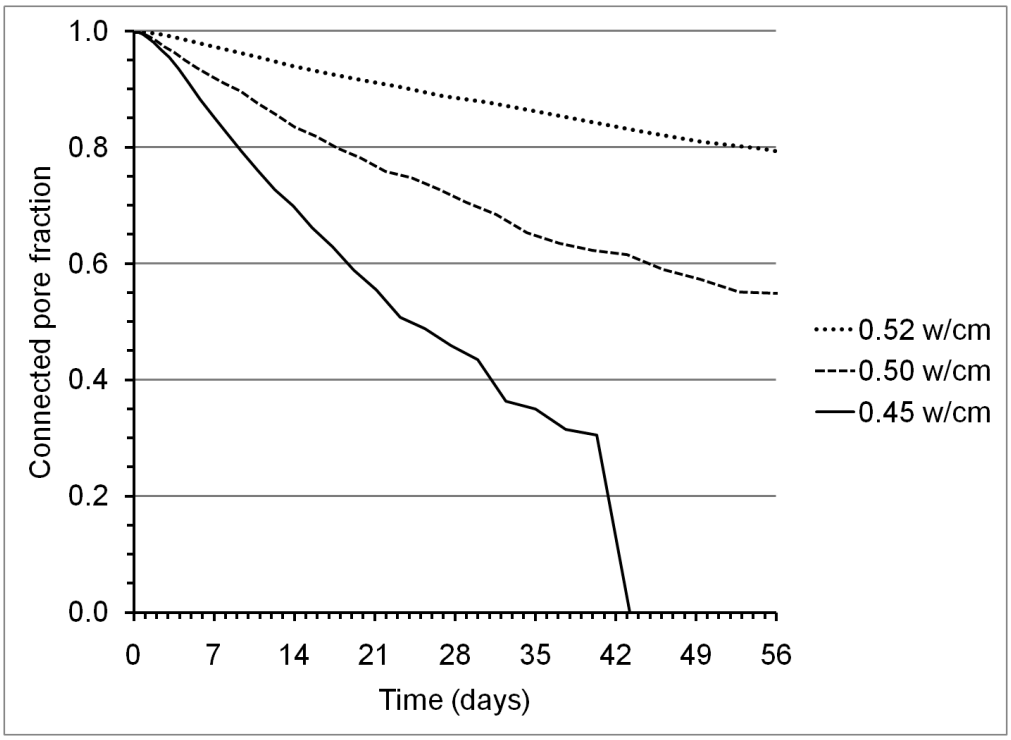

Figure 71: Fraction of connected porosity across the 0.1 mm width of the cube versus time from the hydration models.

5.2.8 Scanning Electron Microscope Examination of Thin Sections

SEM BSE images were recorded from epoxy impregnated polished thin sections from the LO-VR-PC-6SK-45WC, LO-VR-PC-6SK-50WC, and LO-VR-PC-5.5SK-52WC concrete mixtures to make qualitative comparisons to the CEMHYD3D model outputs for the 0.45, 0.50, and 0.52 *w*/*cm* scenarios. Figures 72-74 compare BSE images from the thin sections to slices from the models where the grayscale intensity of phases have been coded to match the BSE images according to the computed phase back-scatter coefficient as described by Thaulow, [2002].

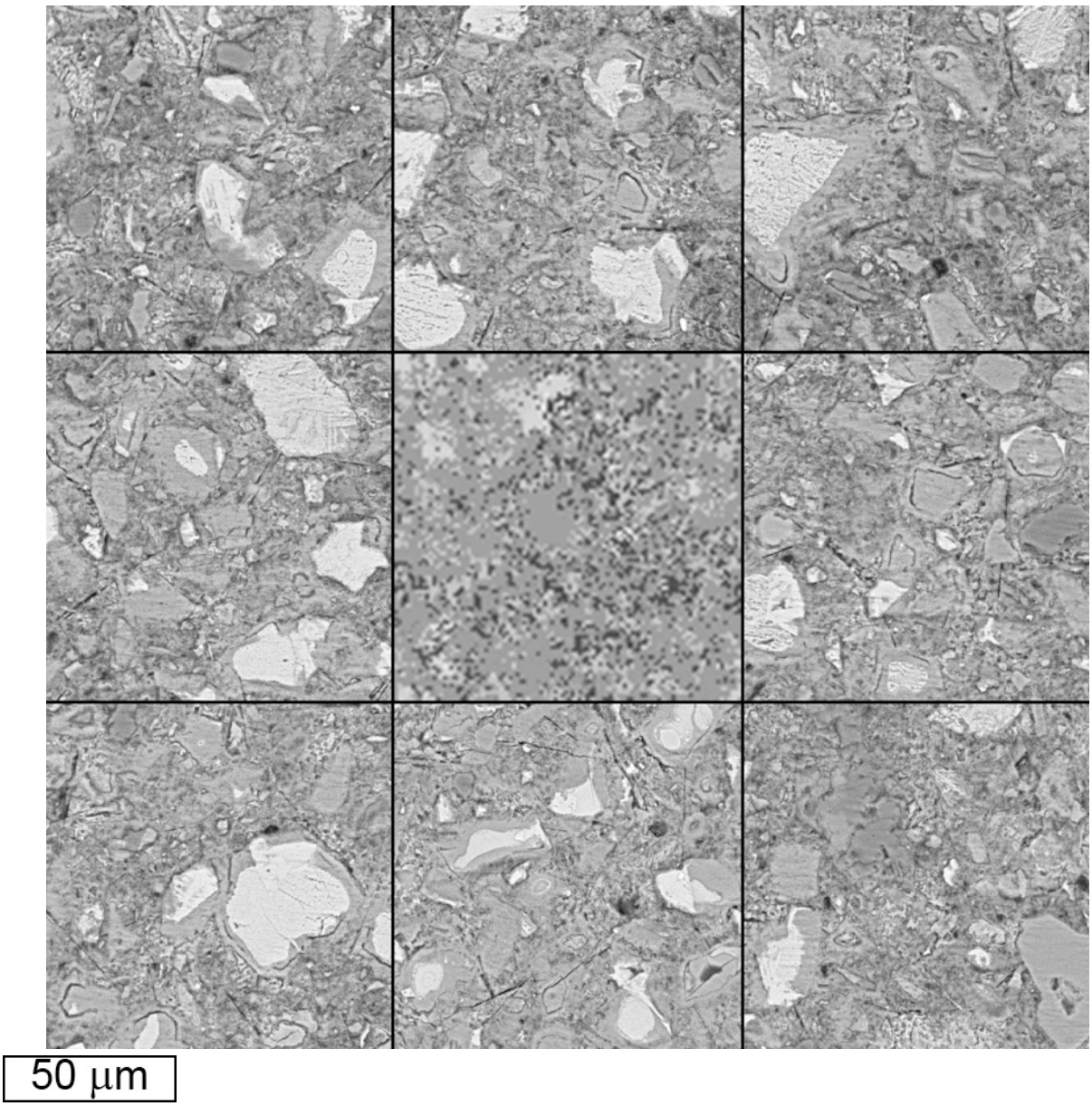

Figure 72: Slice from CEMHYD3D output for 0.45 *w*/*cm* system at 120 days (center tile) compared to BSE images from polished thin sections prepared from 120 day moist-cured 0.45 *w*/*cm* concrete mixture (surrounding tiles).

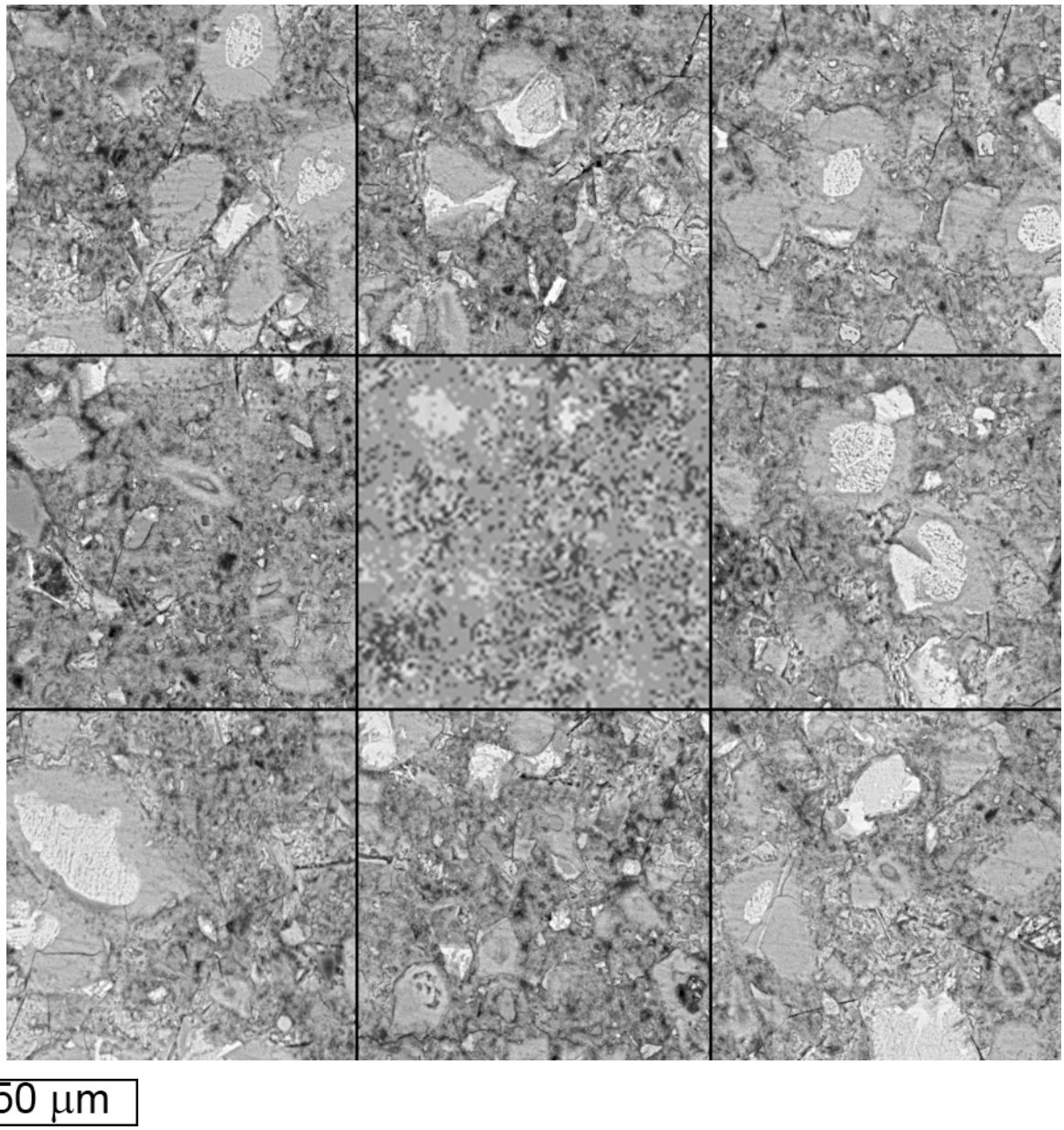

Figure 73: Slice from CEMHYD3D output for 0.50 *w/cm* system at 120 days (center tile) compared to BSE images from polished thin sections prepared from 120 day moist-cured 0.50 *w/cm* concrete mixture (surrounding tiles).

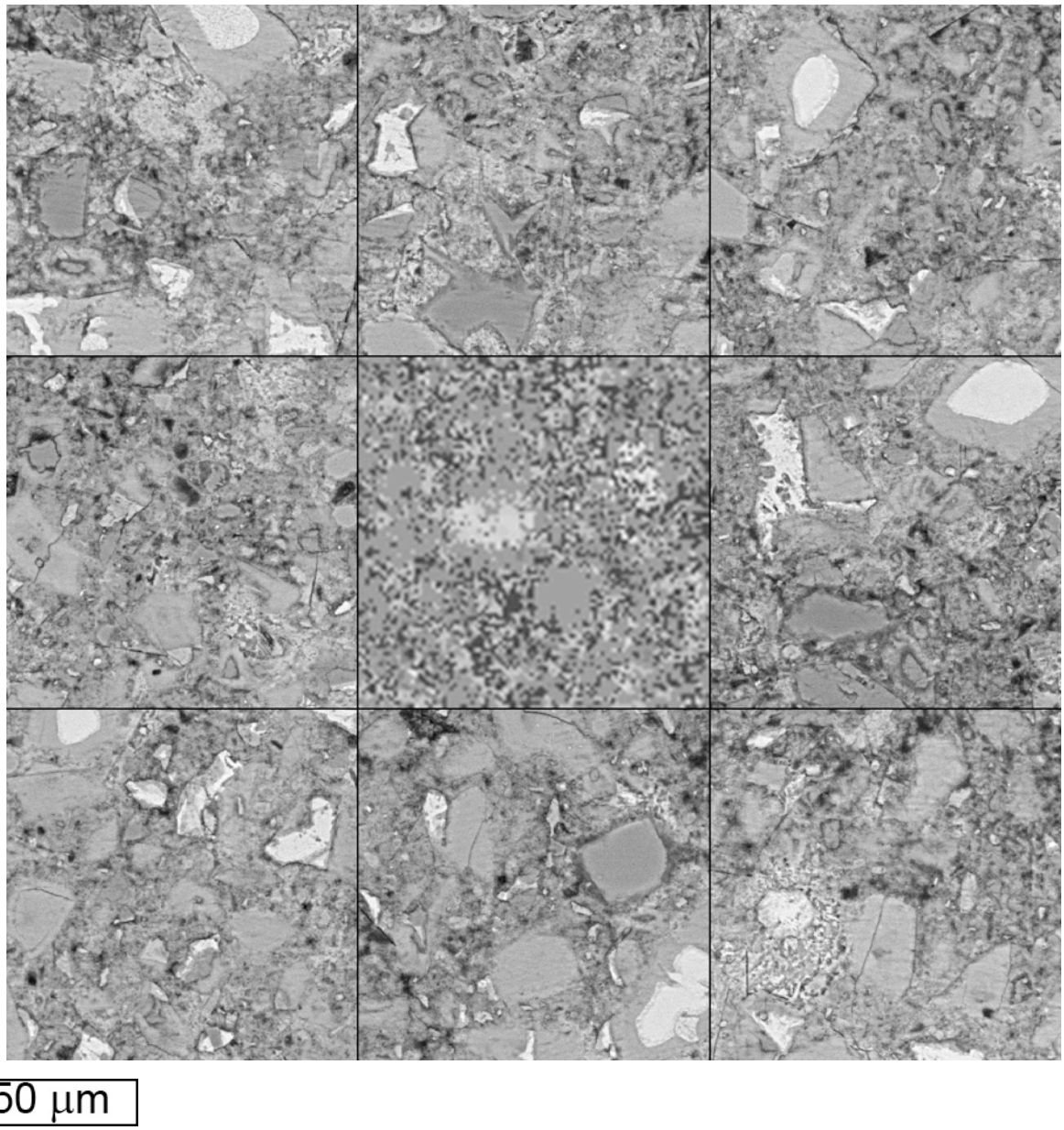

Figure 74: Slice from CEMHYD3D output for 0.52 *w/cm* system at 120 days (center tile) compared to BSE images from polished thin sections prepared from 120 day moist-cured 0.52 *w/cm* concrete mixture (surrounding tiles).