Freeze-casting is a popular method to produce biomaterial scaffolds with highly porous structures. The pore structure of freeze-cast biomaterial scaffolds is influenced by processing parameters but has mostly been controlled experimentally. Three approaches were developed to predict the scaffold pore structure as function of experimental conditions including mold geometry, material and thermal boundary conditions.

First, a mathematical model integrating Computational Fluid Dynamics (CFD) with Population Balance Model was developed to predict average pore size (APS) of 3D porous chitosan-alginate scaffolds and to assess the influence of the geometrical parameters of mold on scaffold pore structure. The model predicted the crystallization pattern and APS for scaffolds cast in different diameter molds and filled to different heights. The predictions demonstrated that the temperature gradient and solidification pattern affect ice crystal nucleation and growth, subsequently influencing APS homogeneity. The predicted APS compared favorably with APS measurements from a corresponding experimental dataset, validating the model. Sensitivity analysis was performed to assess the response of the APS to the three geometrical parameters of the mold: well radius; solution fill height; and spacing between wells. The pore size was found to be most sensitive to the spacing between the wells and least sensitive to solution height. An image processing code was developed as second investigated approach using python and Imagej open source software to analyze the microstructure of the scaffolds including pore size distribution, average pore size and average pore elongation relative to mold geometry. The image processing data were used to correlate the scaffold pore structure with the experimental conditions under which the scaffolds were produced. In the third approach, a deep learning neural network coupled with a support vector machine classifier was used to predict the scaffold pore structure based on CFD results obtained from the first approach. The validated models demonstrate the capability of the methods developed in this study for prediction and optimization of the APS of freeze-cast biomaterial scaffolds that could be applied to other compositions or applications.

Key Terms
Regenerative Medicine, Freeze drying, Porous Scaffold, Pore Size, Computational Fluid Dynamics, Population Balance Model, Solidification, Modeling, Crystallization, Machine Learning, Autoencoder, Pore Size Classification

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The public is welcome to attend.