

CFD MODELING BASED ON X-RAY MICROTOMOGRAPHY RECONSTRUCTION OF LYOPHILIZED PRODUCTS

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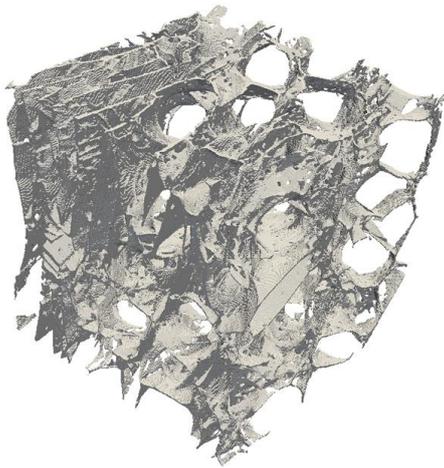
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The governing equations for heat and mass transfer in a porous media, such as the lyophilized cake, depend on structural characteristics of the product. Moreover, knowledge of the internal structure is crucial to better understand the relationship between freezing and within-product heterogeneity, as well as between freezing and the drying behavior of the product being lyophilized.

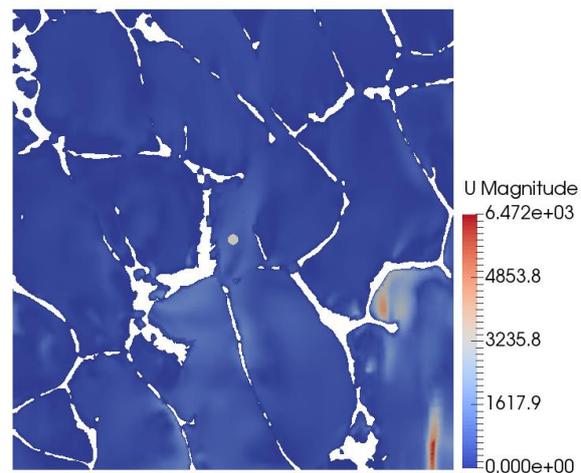
In this work, 3D non-destructive X-ray micro-CT tomography is used to analyze and reconstruct the internal structure of lyophilized samples, and CFD simulations for calculating their structural properties, i.e., porosity, pore diameter, tortuosity, and permeability.

All the simulations were carried out within laminar Stokes' flow, where neither turbulence nor inertial effects are present. While it is true that freeze-drying is characterized by Knudsen (or transition) flow regime, here CFD simulations were only used to calculate the geometrical properties of the lyophilized cake which are independent of the flow regime considered. These properties have then been used by a two-dimensional model to describe heat and mass transfer (under Knudsen regime) during freeze-drying of a frozen solution in a vial.

This method allows a deep knowledge of product structure and a high level of accuracy in predicting mass transport phenomena during drying.



a) Product reconstruction from micro-CT



b) CFD simulation at pore-scale