Development of a Multiphase, Multispecies Droplet Evaporation Model for Optimization of Desiccation Preservation Techniques

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Introduction: Biopreservation deals with the protection and storage of complex biologics such as proteins, lipids, and recently, mammalian cells. One biopreservation technique that is showing great promise for the future use is lyopreservation, where a biologic is placed inside a water droplet with some type of sugar excipient (sucrose, trehalose, etc.) and dried convectively. As the drop becomes more desiccated, glass will form at its surface, preserving the biologic inside. We have observed that solute can build up along the edges of the drop during desiccation (see Fig. 1). This causes the center of the drop to depress and expose the biologic to the ambient air, killing it. Therefore, a large factor in optimizing lyopreservation methods is studying the phenomenon of droplet evaporation as well as designing optimal surface wettability.

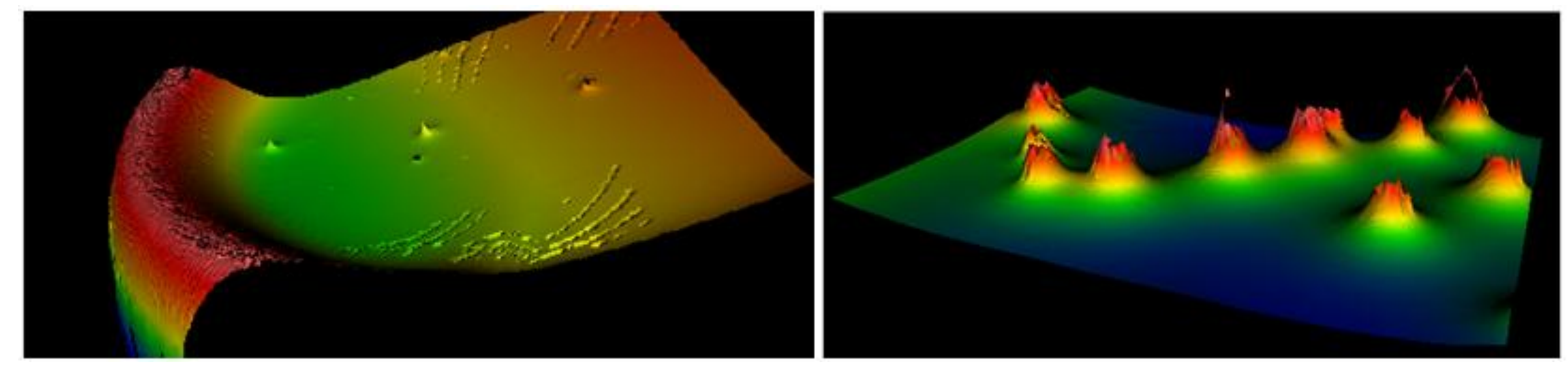

Figure 1. Profilometer scans of dried solution (from [2]). Cells can be seen protruding from center of drop.

The evaporation of a thin film was also simulated using these two physics interfaces. Results of the dry basis moisture content (grams of water / grams of solvent) correlated well with published work (see Fig. 4).

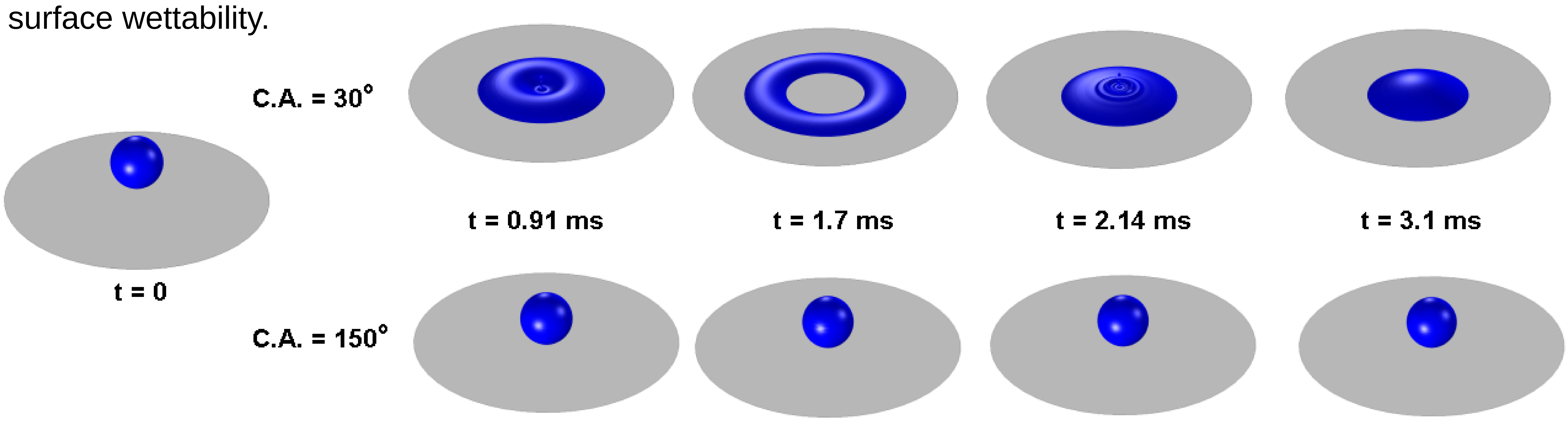

Figure 2. Simulation results of a 250 micron water droplet impacting at 0.1 m/s on substrates with contact angles of 30° and 150° respectively. The Phase Field method was used for the simulations.

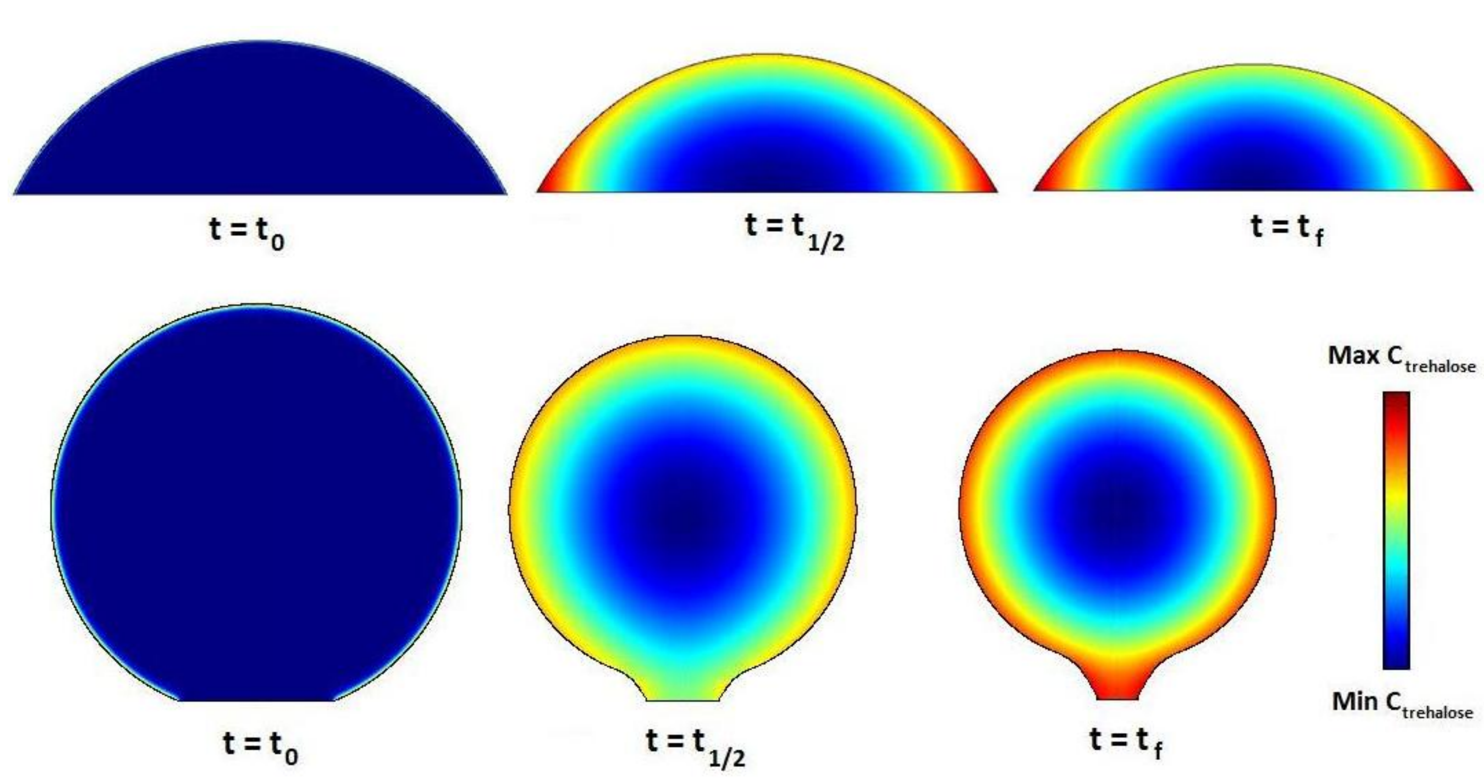

Figure 3. Solute (trehalose) concentration profiles for hydrophilic and hydrophobic geometries.

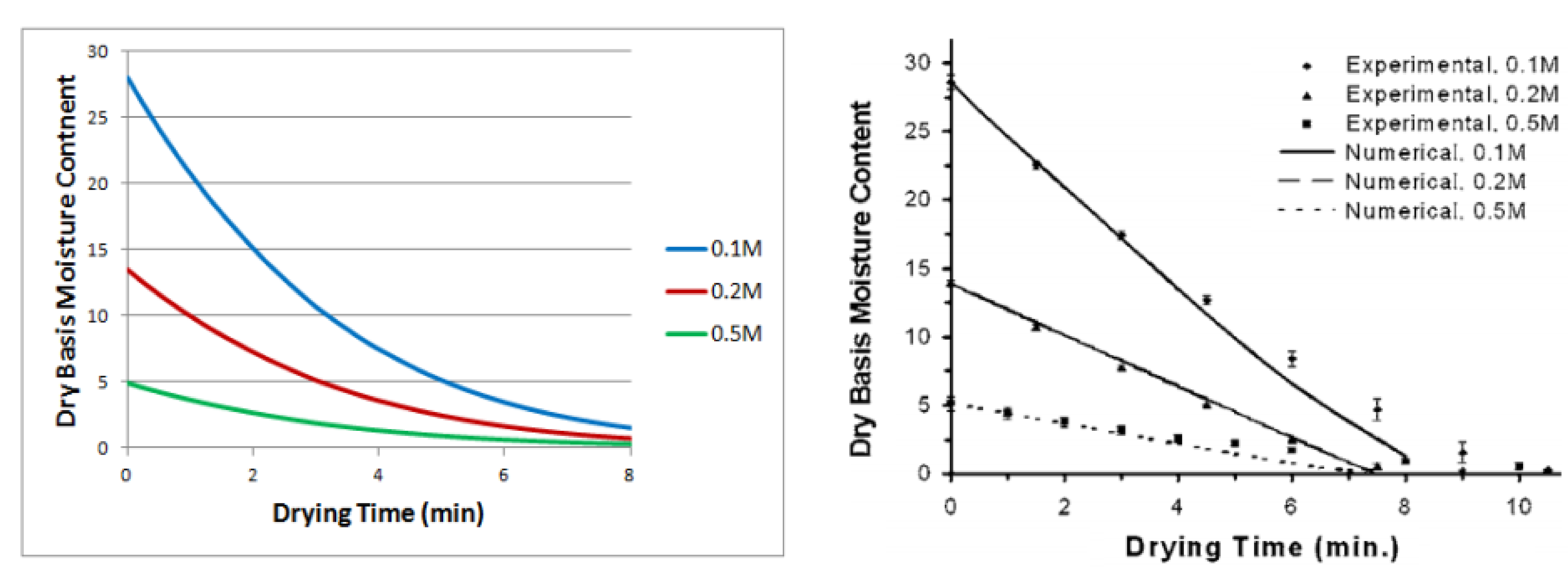

Figure 4. Comparison of drying times for a thin film (COMSOL simulations compared to results from [1])

Model Approach & Current Results: We are currently developing a COMSOL model that couples the Two-Phase Laminar Flow (Phase Field method) and Transport of Diluted Species interfaces to capture the essential transport phenomena during the desiccation process.

Figure 2 shows a water droplet impacting onto surfaces with different contact angles. The equilibrium geometry in these simulations were used as the initial geometry for droplet evaporation tests (see Fig. 3). In these tests, the Transport of Diluted Species interface captured the water and sugar excipient concentration profiles. The Deformed Geometry interface was used to account for the change in mass during desiccation.

Conclusions: The results thus far have instilled a solid foundation needed for the continuation of this study. More tests will be performed using the Two Phase Laminar Flow, Transport of Diluted Species, and eventually Heat Transfer in Fluids interfaces. A fully coupled model will lead to a more complete understanding of the thermophysical state around the biologic within the drop during desiccation. Once the final model has been validated, it will be used for designing optimal droplet evaporation, wetting properties, and humidity conditions. This would, in turn, assist in optimizing desiccation protocol for biopreservation techniques.

References:

1. B. Chen, A. Fowler, S. Bhowmick, Forced and natural convective drying of trehalose / water thin films: implication in the desiccation preservation of mammalian cells, Journal of biomechanical engineering, 128, 335-346 (2006)
2. Oliveira, M. (2012) Biophysical Impact of Trehalose in Mammalian Cell Desiccation Preservation: Convective Desiccation of a Sessile Droplet (unpublished Master's thesis). University of Massachusetts Dartmouth. North Dartmouth, MA

Excerpt from the Proceedings of the 2013 COMSOL Conference in Boston