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

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## Abstract

Biopreservation deals with the protection and storage of complex biologics such as proteins, lipids, liposomes, and recently, mammalian cells. Since the field of reproductive technology is rapidly growing, there is a growing need for continual improvements in the techniques used for biopreservation. One such method 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. Traditional methods such as cryopreservation (freeze drying) are expensive and carry a variety of difficulties, and lyopreservation appears to offer promise as a simpler method of biopreservation. A large factor in optimizing this method is studying the phenomenon of droplet evaporation.

This work is currently in its developmental stages. The 2D-axisymmetric model utilizes the two phase laminar flow (phase field method) interface coupled with the transport of diluted species interface to simulate a suspended pure water droplet evaporating in space. The absence of gravity simplifies the problem greatly and allows the evaporation physics to be more objectively studied. Sugar excipients have not yet been added but since biologics are primarily comprised of water, the importance of studying the evaporation of pure water droplets remains. Temperature is assumed to be constant, hence heat transfer is negligible. Conservative forms of the equations are used for both the fluid dynamics and mass transfer physics. Following the study on the suspended drop, the model shall be extended to an evaporating sessile droplet with multispecies transport.

A preliminary study has been performed using two-phase laminar flow physics (Phase Field and Level Set methods) for falling droplets onto substrates with varying hydrophobicity. These simulations behaved realistically, capturing the physics involved. The current study on a suspended drop and future study on a sessile drop will eventually lead to a full coupling of all of the transport phenomena present during droplet evaporation. This 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 could be used for designing optimal droplet geometry, wetting properties, and humidity conditions. This would, in turn, assist in optimizing desiccation protocol for biopreservation techniques. The final model could also serve as a

template for researchers interested in using COMSOL Multiphysics® for simulating their multiphase, multispecies problems.