

Modeling Porosity Development during Drying of Liquids and Slurries

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Project Objective:

The project aims to provide an accurate description of the micro-scale physical phenomena that contribute to the formation and evolution of bubbles in gas-saturated slurries during foaming spray drying. These phenomena include bubble nucleation and growth driven by pressure depletion, as well as capillary action combined with liquid flow resistance, dissolved gas transport, vapor diffusion, and the liquid-to-gas phase change. Our approach is to formulate discrete rules for these phenomena and progressively integrate them into a three-dimensional pore network model, in which the complex void space of a single slurry droplet is represented as a regular lattice of pores. This systematic and modular framework will ultimately enable us to gain fundamental insights into the foaming behavior of a single slurry droplet and its impact on internal morphology (e.g. porosity) development and drying kinetics.

Approach:

Our approach for modeling the drying of a single slurry droplet is to conceptualize it as three-dimensional networks composed of pores and particles, with particles occupying the space between the pores. Initially, the pores are filled with a liquid supersaturated with inert gas, and their sizes are distributed according to a probability density function. Bubble nucleation occurs at small cavities located on the pore walls, which also vary in size. Under steady-state conditions, the growth of each bubble is governed by the balance between gas pressure inside the bubble, liquid pressure, and capillary pressure. In each growth step, dissolved gas is transported toward the bubble interface, driven by the concentration gradient between the bubble surface and the surrounding liquid, while simultaneously diffusing through the pore network. As bubbles grow, they invade neighboring pores following imbibition rules, thereby altering the liquid distribution (but not yet the local pore structure itself). These changes affect the evaporation behavior, which is modeled as external evaporation described by gas-side diffusion across a boundary layer, and internal evaporation driven by capillary-controlled liquid transport. By discretely formulating and coupling these interdependent mechanisms, we provide a detailed kinetic view of the interplay between evaporation and bubble formation during the drying of single slurry droplets.

Recent Results:

Our previously developed discrete rules for bubble growth and expansion have been adapted and coupled with rules for local evaporation and liquid redistribution in a threedimensional pore network model to study their combined impact on the drying kinetics of slurry droplets. Simulations that account for both gas diffusion and evaporation indicate a vertical concentration gradient, with lower gas concentrations near the droplet surface and higher concentrations toward the bottom. This gradient affects bubble formation: surfaceconnected bubbles grow more slowly due to smaller concentration differences. Comparing simulations with and without bubbles shows significant differences in drying behavior. The presence of bubbles reduces overall drying time (by 23% for a network dimension of $20 \times 20 \times 20$ pores) by enhancing evaporation rate. In the bubble-containing simulation, drying proceeds with an extended constant-rate period sustained by internal bubble growth, which drives liquid displacement toward the surface. Under the specific network configuration and boundary/initial conditions used in our simulations, the droplet surface remains wet at a network saturation of 0.5 in the bubble simulation, while it has already dried in the simulation without bubbles – resulting in a higher drying rate for the former (Fig. 1). As saturation decreases below 0.2, the drying rates of both simulations converge as bubbles either collapse or connect to the external environment. Further analysis shows a more uniform local saturation distribution in the drying simulation with bubbles, whereas the non-bubble drying simulation displays a gradient with increasing saturation from surface to bottom. These results – while specific to the simulated network and conditions - demonstrate that internal bubble formation can modify and intensify the drying process in slurry droplets.

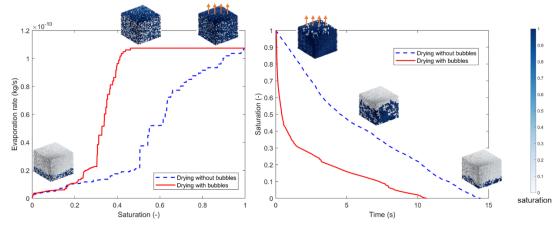


Figure 1: Drying kinetics and saturation distributions from pore network simulations with and without bubbles. Results are shown at different network saturation levels during drying. Simulations were performed on a $20 \times 20 \times 20$ pore network, with evaporation occurring from the top. Liquid is pure water, and drying was modeled under room conditions.

Next Steps:

So far, the pore network model has been developed and applied to study bubble dynamics and the drying behavior of slurry droplets. The consideration of capillary forces acting on the solid phase, which are expected to influence the final product morphology (both internally and at the surface) is planned in future work.