IFPRI Project Abstract

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 evaporative drying. These phenomena include heterogeneous nucleation and bubble growth, as well as capillary action coupled with liquid flow resistance, dissolved gas transport, vapor diffusion, and 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. This systematic method enables us to study the impact of slurry characteristics and process parameters on porosity development during the drying of slurries.

Approach:

The gas-saturated liquid medium is viewed as containing a volatile solvent with dispersed solid particles. This medium is conceptualized as a three-dimensional network consisting of both pores and particles, with particles filling the spaces between the pores. Initially, the pores contain a liquid that is supersaturated with gas, and their sizes follow a probability density function. Nucleation sites, where bubbles form, are located in small cavities on the walls of the pores, and their sizes also vary. Under steady-state conditions, the growth of each bubble depends on the balance of gas pressure inside the bubble, liquid pressure, and capillary pressure. During each bubble growth step, the transport of dissolved gas is driven by the concentration gradient between the bubble surface (liquid-gas interface) and the gas concentration in the surrounding liquid. Future modeling steps will include the evaporation of solvent from the pores, and the transport of solvent vapor in air-rained pores, and the migration of bubbles to adjacent pores.

Recent Results:

Discrete rules formulated for describing bubble nucleation and growth are incorporated into a three-dimensional pore network model. Multiple simulations are conducted using a relatively small pore network (5×5×5) to study the influence of initial liquid pressure on the evolution of gas concentration, as well as the distribution of bubble sizes and the evolution of bubble density. In these simulations, the radii of the cavities, where bubble nuclei may form, follow a normal size distribution, with a mean radius of 6 nm and a standard deviation of 3 nm. The network is initially filled with gas-saturated liquid at a pressure of 200 bar. At the cavities where liquid-gas interfaces (menisci) form, the liquid pressure is balanced by gas pressure and capillary pressure. With a given liquid pressure (in this case, 200 bar) and a known capillary pressure under equilibrium conditions, the gas pressure and concentration inside the cavities are determined. Upon a pressure drop from 200 bar to 1 bar, the previous pressure equilibrium is disturbed, leading to a new steady state where the gas pressure inside the bubble is once again balanced by liquid pressure and capillary pressure. This state is considered the bubble nucleation phase. The bubble gas pressure and concentration are determined using the ideal gas law coupled with the pressure balance equation. In our case, during the pressure drop from 200 bar to 1 bar, 73% of the cavities can initiate bubbles, with a minimum radius of 7.29 nm (Fig. 1a). Due to concentration differences between the gas-liquid interfaces and the gas concentration in the pores, gas molecules transport is driven by the diffusion process. Molecules may diffuse into the bubble, leading to bubble growth, while others may dissolve into the liquid, resulting in bubble shrinkage. A time step of 0.1 ms is chosen. As the diffusion process proceedes, the bubble continues to grow until gas molecule equilibrium is reached. Figures 1b and 1c show the state of the bubble size and gas pressure inside the bubbles after nucleation at 0.1 ms and 10 ms, respectively.

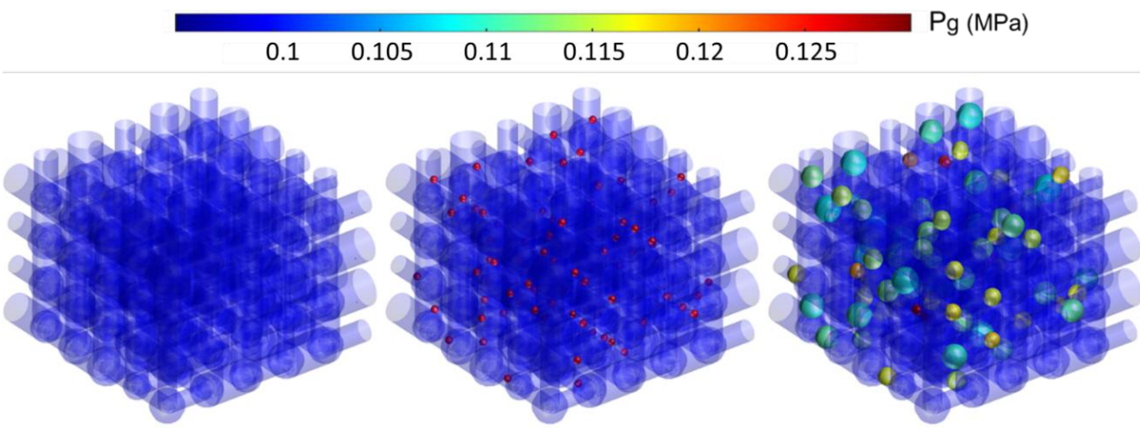

Figure 1: Bubble distribution following a liquid pressure drop from 200 bar to 1 bar, showing bubble size and gas pressure at (a) 0 ms, (b) 0.1 ms, and (c) 10 ms after nucleation.

Next Steps:

Until now, bubble growth has been described as occurring due to an abrupt pressure drop in the liquid phase, with no consideration for the volume of liquid displaced by the growing bubble. The model will be expanded by including the evaporation of the liquid, as well as the transport of both liquid and vapor, and how these phenomena affect the local gas concentration and redistribution of liquid caused by bubble growth.