



Encapsulating and Protecting Delicate Electronics

The chemical engineering and modeling underpinning polymeric foams encompass a complex interplay of challenges

Sometimes, in researching a topic that appears from a distance to be reasonably simple and straightforward, one is ultimately compelled to reconsider that judgment as naïve. The topic of foams turns out to be just such an instance.

Whether it's the packaging foam in your UPS shipment or the protective enclosure for a delicate bit of electronics within a weapon or other critical system—a so-called chemically blown (expanded) foam is produced by a liquid mixture of organic molecules poised to undergo a set of chemical reactions that will first, generate a gas (often CO_2) that creates bubbles and expands the liquid into a foam, then stabilize and harden (or “cure”) that foam into a solid by inducing the forming of chemical bonds that complete the polymer of which the solid foam is ultimately composed. Whether epoxy-based or polyurethane-based—the two predominant polymeric chemistries—the goal is a solid of a specific shape with a small and uniform bubble size (fig. 1) that resists compression, able to tolerate external pressure and other forces while protecting some structure that it encloses or surrounds.

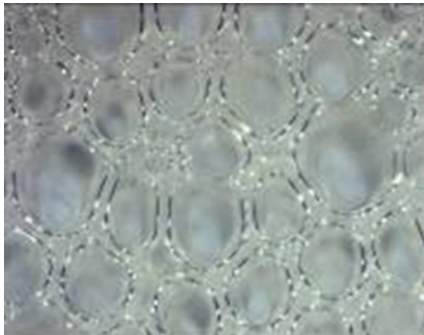


Figure 1. Micrograph of an epoxy foam illustrating its structure as a collection of bubbles trapped within a polymeric framework.

In addition, for structural foams, the dimensional stability, or lack thereof, with aging must be understood. Foams can also be physically blown using a volatile blowing agent, in which case, the foaming reaction is initiated/controlled by altering

some physical parameter, such as temperature or pressure.

Foams play a role in several areas of Sandia's mission space, but none quite as important as protecting delicate electronics from physical insults, thereby guaranteeing their ongoing functionality. Although they have successfully done so for decades, legacy foams suffer from certain drawbacks, including the inclusion of chemistry that can immunologically sensitize

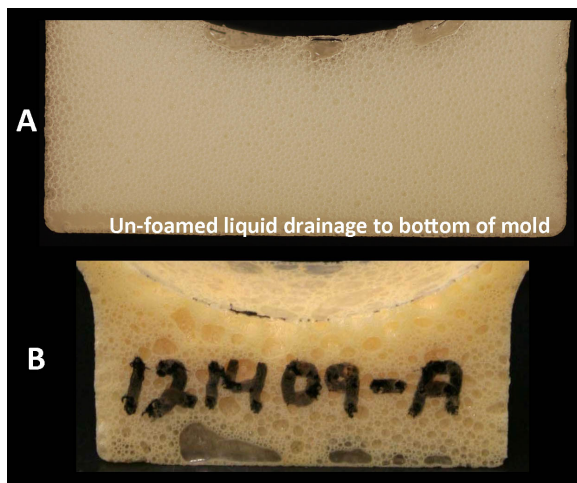


Figure 2. A: Drainage of unfoamed liquid at the bottom of a mold because of high density and a delay in curing. B: Overly large bubbles formed during curing of a lower-density foam.

workers to re-exposure (a form of allergic reaction), as well as being difficult to remove once in place. Additionally, physically blown foams employed in certain Sandia applications, are more difficult to control.

Given these circumstances, the Sandia LDRD program funded research into a study of alternative foam approaches from both a chemical engineering and a modeling perspective. If anything, this project validated the view of Sandia chemist Mat Celina that foams are “challenging materials where everything has to be perfect.”

A foam takes its shape by being poured or forced under pressure into a mold, where, as a reacting liquid that expands as gas bubbles forms, it must fill all spaces—sometimes extremely narrow ones. Then, just at the right moment, the foaming process is stopped, and the foam cures by polymerizing the liquid into a solid, such that one creates a homogeneous foam with evenly spaced bubbles of a consistent size, and therefore consistent protective properties as it forms around a delicate bit of electronics as defined by the mold’s size and shape. (This “right moment” description is idealized, given that, in real situations, the foaming and curing reactions are occurring during the same time window). If this curing occurs too slowly and/or the foam-liquid’s density is too high, gravity can drive un-bubbled liquid to the bottom of the mold (fig. 2A). In other situations, such as in delayed curing of foams of lower density, bubbles can merge together creating an unevenness in bubble size and spacing (fig. 2B). This phenomenon known as coalescence, where bubbles merge together, and Ostwald ripening by which gas moves from smaller to larger bubbles, also can contribute to a lack of homogeneity in bubble size and distribution. Such undesirable attributes can leave a foam with weak spots, and thus, with inadequate protective properties, inadequate resistance to compression and other stresses. Conversely, if the curing (polymerization to a solid) occurs too rapidly, prematurely eliminating liquid properties (rheology) of the foaming chemicals, the foam will fail to fill all spaces in the mold—particularly very small, narrow spaces (see fig. 3), leaving voids without foam, a clearly undesirable outcome.

PI Lisa Mondy and her LDRD research team studied a diversity of new routes to such chemical foaming with production of CO₂, chemistries that would reduce toxicity and bring a greater measure of control over and understanding about the

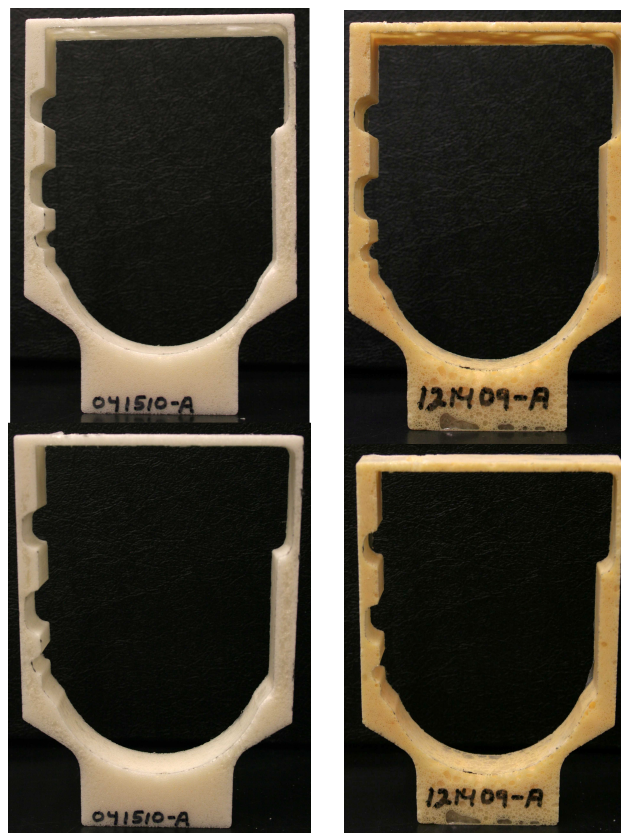


Figure 3. Comparison of foams within mold, relatively homogeneous foam, at left, compared to foam with voids (at right) a result of bubble coarsening. Filling of narrow passageways such as the top horizontal beam of the mold is always difficult, and is somewhat easier if foam curing can be delayed slightly to maintain foam liquidity.

foaming and curing processes. With a background in multiphase flow, Lisa began her Sandia career with a study of geothermal drilling foams, and after several successful proposals to study the flow of suspensions, she began working with Rekha Rao in modeling particle migration, and this collaboration brought the pair to encapsulation foams through some work with Sandia staff encapsulating critical components with particle filled epoxies. Assisted by campaign and Advanced Simulation and Computing (ASC) funding, they began to model extant stockpile foams. In the process, the problems they encountered provoked creative ideation that led to funding of the LDRD project and collaboration with creative material chemists like Celina and manager Jim Aubert, a chemical engineer who worked on foams early in his career. Celina, whose background lay in applied polymer science and materials optimization had previously worked with the Kansas City Plant (KCP) on reliability issues in foams processing.

As part of the LDRD, the team's modeling of the existing chemistry (fig. 4) was guided by the long-term goal of extending this model to whatever chemistry appeared to be the most propitious. Ultimately, the intent was to render the model adaptable

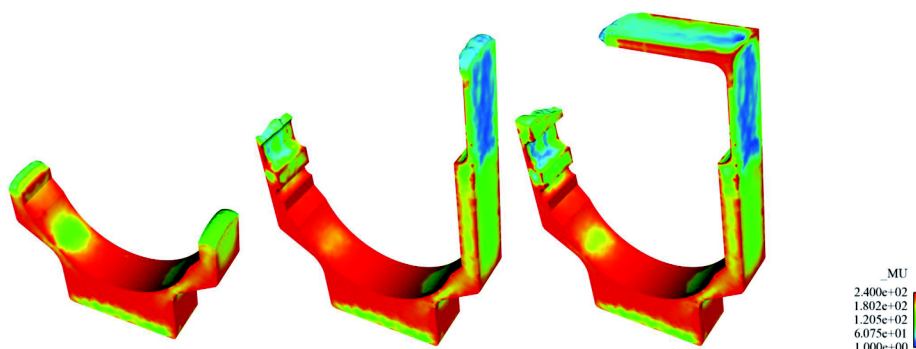
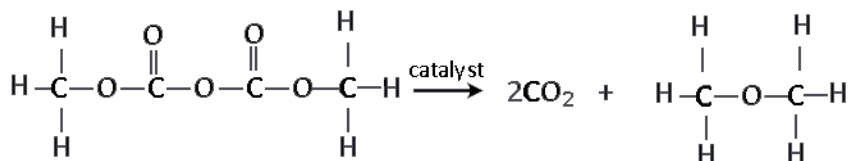


Figure 4. Computational modeling of foam injection in the mold. The foam is modeled as a shear-thinning material, ignoring irreversible effects of bubble breakage. In large sections, the viscosity behaves as a Newtonian fluid and in small sections, the viscosity thins to a quarter of that value.

to diverse chemistries, a breakthrough engineering model that did not previously exist. With respect to the experimental chemistry, the goals of the project were to move toward the best aspects of existing foams without their liabilities, and to project potential future needs of life extension programs. This aspect of the project involved a collaboration with KCP, a collaboration that is ongoing.

After studying numerous methodologies for generating CO₂ bubbles, the project developed novel, stable epoxy foams using a liquid epoxy anhydride system that generates CO₂ bubbles through the decomposition of tert-butoxycarbonyl anhydride, the reaction generally representable as follows:



One goal was to develop a system in which the foaming and curing reactions were more separable than the equivalent reaction in extant polyurethane-based foams, in which the foaming and curing reactions are intrinsically coupled to a greater extent. Such coupling makes it more difficult to maintain the foaming chemistry in a liquid state in order to fill difficult narrow passageways within a mold, the existing foam chemistry characterized as “unforgiving.” “Foams are tough systems; all the chemistry tends to be happening together,” says Celina. This was especially problematic in attempts to use spectroscopic signatures to follow the kinetics of individual reactions. Because of cross-talk in reaction chemistries, isolating a clear infrared (IR) spectroscopy signal for the rate of CO₂ evolution proved to be virtually impossible, particularly since additional CO₂ was evolved during curing, subsequent to that produced in foaming. Hence, despite a system, that did achieve a greater separation between foaming and curing, this was not complete, mostly because the cure process involves very effective chemistry that cannot be completely delayed.

Physical compression tests and shear tests validated the novel foam as falling within the desired range of values necessary for use in actual situations, although future requirements may demand new performance metrics from all foams. This and other issues would likely benefit from the ability to extend the current model to a wider range of chemistries. To that end, follow-on funding for ongoing model development has come from ASC as well as from the weapons program itself. The model is currently being used at KCP to help design molds and reduce defects in encapsulated parts.

Ongoing support for the polymer chemistry and processing aspects of the research, for qualification in future weapon’s systems, would appear to be a judicious investment. Given the uncertainty regarding future needs and the consequent desirability for flexibility in being able to generate novel foams for critical life extension initiatives, such research looms as an important component for that future. Clearly, qualifying a new material in this particular arena is a rather difficult proposition. Part of the reason is the nature of the materials themselves. Starting from the non-intuitive proposition that generating a gas within a liquid ends up with the formation of a solid, foams—even with a high degree of knowledge and understanding about the individual chemical reactions involved—manage to behave somewhat differently than anticipated. A system that, at first glance, seems simple and straightforward, upon deeper examination, proves to be fantastically challenging. These initiatives that foster greater scientific and technological understanding should ultimately contribute to key national security requirements important to several Sandia missions.

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