A CONFORMAL DECOMPOSITION FINITE ELEMENT METHOD FOR POLYURETHANE FOAM EXPANSION

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Abstract - We are developing computational models to elucidate the expansion and dynamic filling process of a polyurethane foam, PMDI. The polyurethane of interest is a chemically blown foam, where carbon dioxide is produced via the reaction of water, the blowing agent, and isocyanate. The isocyanate also reacts with polyol in a competing reaction, which produces the polymer. A new kinetic model is implemented in a computational framework, which decouples these two reactions. The model predicts the polymerization reaction via condensation chemistry and foam expansion kinetics through a Michaelis-Menten approach. Both reactions are exothermic and temperature dependent. The conservation equations, including the equations of motion, an energy balance, and two rate equations for the polymerization and foaming reactions, are solved via a stabilized finite element method. The rheology is determined experimentally and is assumed to follow a generalized-Newtonian law where it depends on the degree of cure and temperature, but is not viscoelastic. The conservation equations are combined with a novel free-surface algorithm, termed the conformal decomposition finite element method (CDFEM), to determine the location of the foam front as it expands over time. CDFEM combines a level set method to track the gas-foam interface and then adds mesh conformally at this interface to allow for easy application of interfacial physics such as capillary pressure jumps, creating a sharp-interface. The model predicts the velocity, temperature, viscosity, free surface location, and extent of polymerization of the foam. In addition, it predicts the local density and density gradients based on the Michaelis-Menten kinetics of foam expansion. Results from the model are compared to experimental flow visualization data and post-test CT data for the density.

Keywords: polyurethane foam, kinetics, finite element method, level set, conformal decomposition

Introduction

We are developing computational models to elucidate the expansion and dynamic filling process of low density polyurethane foam, polymeric methylene diphenyl diisocyanate (PMDI-4). Here the “4” indicates the density of the foam is 4 lb/ft^3. The polyurethane of interest is chemically blown foam, where carbon dioxide is produced via the reaction of water, the blowing agent, and isocyanate. The isocyanate also reacts with polyol in a competing reaction, which produces the polymer. An example of a free rise sample of the PMDI is shown in figure 1.

Figure 1. PMDI has a short pot-life: models can help reduce defects and improve filling process**.**

PMDI has a short pot-life, meaning that it cures quickly. In addition, the foam expansion due to CO_2 generation occurs concurrently to the polymerization reaction. Models are needed to help reduce defects such as voids, density gradients, exotherms, and incomplete filling and to optimize processing parameters such as vent and gate location, oven temperatures and filling rates.

A new kinetic model is implemented in a computational framework, which decouples the curing and foaming reactions. The model predicts the polymerization reaction via condensation chemistry and foam expansion kinetics through a Michaelis-Menten approach. Both reactions are exothermic and temperature dependent.

A continuum mechanics approach is taken to solving the foam blowing problem, coupling conservations to the rate equations. The resulting system of equations is solved via a stabilized finite element method that is coupled to a novel moving boundary algorithm to determine the location of the foam free surface as a function of time. The new algorithm is a hybrid Eulerian-moving mesh approach termed conformal decomposition finite element method (CDFEM) [1].

In previous papers, we focused on developing engineering models of foam expansion for polyurethane and EFAR foams, respectively [2, 3]. The models were relatively complete, except that the density was used as an input parameter instead of predicted as part of the model, following ideas from Seo et al [4].

In this paper, we focus on the details of a computational model that predicts the density of the foam as it evolves. The details of the experiments used to inform and populate the model are available in a companion paper [5]. The paper is organized in the following manner. In the first section we discuss the equations of motion and constitutive equations for the foam chemo-rheology. In the next section, we briefly describe the numerical methods. Results from the model are compared to experimental flow visualization data and post-test CT data for the density. We conclude with plans for future work.

Equations

The continuity equation is written to emphasize the change in density as the source of foam velocity generation, where v is the mass-averaged velocity and ρ is the foam density. Here we no longer have an incompressible material, but rather one with an evolving density and density gradients.

$$\frac{\partial\rho}{\partial t} + v\bullet\nabla\rho = -\rho\nabla\bullet v \qquad (1)$$

Conservation of momentum takes into account gradients in the fluid stress, τ, and pressure, p, as well as gravitational effects. Note that gravity is applied to the homogenized foam material and does not take into account the buoyancy differences between the polymer and the gas bubbles that may result in creaming.

$$\rho\frac{\partial v}{\partial t} + \rho v\bullet\nabla v = \nabla\bullet\underline{\underline{\tau}} - \nabla p + \rho\underline{g} \qquad (2)$$

The stress tensor has a generalized Newtonian shear viscosity, in addition to a generalized Newtonian bulk viscosity. The bulk viscosity is associated with the fact that the divergence of the velocity field is non-zero and we have a dilatational flow [7]. The bulk viscosity term produce only normal stresses and not shear stresses.

$$\underline{\underline{\tau}} = \eta(\nabla v + \nabla v^t)) - (\frac{2}{3}\eta - \kappa)(\nabla\bullet v)\underline{\underline{I}} \qquad (3)$$

The shear viscosity, η, can be a function of temperature, cure, and gas fraction as discussed elsewhere [3,5].

$$\eta = \eta_{00}\exp\left(\frac{E_a}{RT}\right)\left(\frac{\xi_c^b - \xi^b}{\xi_c^b}\right)^q \exp\left(\frac{\phi_g}{1-\phi_g}\right) \quad (4)$$

where ξ is the extent of reaction for the polymerization reaction, ξ_c is the gel point, E_a is the activation energy, and η_{00} is the uncured viscosity at a reference temperature T_0, and b and q are exponents for the model, and ϕ_g is the gas volume fraction. An expression for the bulk viscosity κ for non-dilute foams was discussed elsewhere [3].

$$\kappa = \frac{4}{3}\eta_{polymer}\frac{(1-\phi_g)}{\phi_g}. \qquad (5)$$

The energy in the system must also be tracked to determine the temperature variations from various sources including oven heating and exothermic polymerization reactions. The energy equation has a variable heat capacity, C_p, and thermal conductivity, k, both of which depend on the gas volume fraction.

$$\rho C_p\frac{\partial T}{\partial t} + \rho C_p v\bullet\nabla T = \nabla\bullet(k\nabla T) + S_{rxn} \quad (6)$$

Polymerization Kinetics

Once the extent of reaction and activation energy are determined, the reaction kinetics (e.g. rate constant and order of reaction) can be obtained by fitting the equation below to the numerically differenced data. The condensation chemistry form of the extent of reaction works well for polyurethane polymerization.

$$\frac{d\xi_{cure}}{dt} = k_0 e^{\Delta E/RT}\left(1-\xi_{cure}\right)^n \qquad (7)$$

Where k_o is the rate coefficient, ξ_{cure} is the extent of reaction, t is time, T is the temperature in Kelvin, ΔE is the activation energy, R is the universal gas constant, and n is the reaction rate.

Density Prediction Model

In previous work, we fit the foam density to experimental data based on a time- and temperature-dependent density model. This was a useful engineering approach to allow us to predict the filling behavior of the foam. Here, we follow a more science-based approach where the model predicts the density from the concentration of carbon dioxide gas produced. The gas is produced via the reaction of water with isocyanate to produce carbamic acid, which then decomposes to form carbon dioxide. We found that it is possible to decouple the foaming and polymerization reaction, even though they both use isocyanate. We hypothesize that this is because isocyanate is in excess, especially at early times.

We define α as the extent of the conversion of water to CO_2. α_{max} is the maximum conversion for a universal correlation for foams with different water content and is temperature dependent. We follow a Michaelis-Menten form of the first order kinetics that fits the shape of our data [6].

$$\frac{\partial\alpha^*}{\partial t} = \frac{k(1-\alpha^*)^n}{(1-\alpha^*)^m + M}, \quad \alpha^* = \frac{\alpha}{\alpha_{\max}} \qquad (8)$$

Two rate coefficients, k and M, are used and both follow Arrhenius type temperature dependence.

$$k = A_1 \exp(-E_1 / RT)$$
$$M = A_2 \exp(-E_2 / RT) \qquad (9)$$

The moles of gas, n_{CO_2}, can be calculated from α and α_{max}

$$n_{CO_2} = n^{i}{}_{CO_2} + \alpha^{*} \alpha_{\max} n^{\max}{}_{CO_2}$$
$$\alpha_{\max} = f(T) = \alpha_1 T(K) - \alpha_1 \qquad (10)$$

The volume fraction of gas, ϕ(t), is related to the moles of carbon dioxide produced, the density of the gas, and the molecular weight.

$$\phi(t) = \frac{n_{CO_2} MW_{CO_2} / \rho_{CO_2}}{n_{CO_2} MW_{CO_2} / \rho_{CO_2} + V_{liquid}} \qquad (11)$$

The density of foam, ρ_{foam}, is now a predicted from the model.

$$\rho_{foam} = (\rho_{CO_2} - \rho_{liquid})\phi(t) + \rho_{liquid}$$
$$\rho_{CO_2} = MW_{CO_2}(p / RT) \qquad (12)$$

Numerical Method

Because our foam expands over time, filling the mold, we need a moving boundary algorithm to track the location of the free surface. Many free surface algorithms exist from Eulerian methods such as volume of fluid and level set methods to moving mesh methods. Here we use a novel method termed CDFEM, which is a hybrid of level set methods and moving mesh methods.

In CDFEM, a background, non-conformal mesh is decomposed into elements that conform to the boundaries of the fluid domains, which are described in terms of a level set field. Enrichment takes place by adding nodes where the edges of the background mesh intersect the level sets. By dynamically adding nodes and associated degrees of freedom on the moving interfaces, weak and strong discontinuities are described with standard finite element shape functions. See Figure 2 for a cartoon describing the algorithm. The example is shown for a background mesh of quadrilateral elements, which are then enriched with the addition of triangular elements. In the actual algorithm, only triangular elements are used in 2D and only tetrahedral elements are used in 3D.

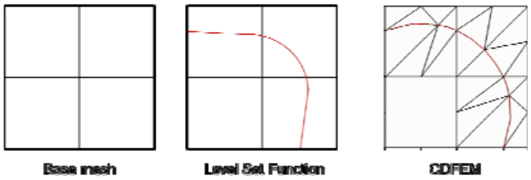

Figure 2. The CDFEM algorithm begins with a base mesh and then creates mesh on the interface location, as defined by the level set. As the interface moves, the old CDFEM mesh is deleted and new interface mesh is added. A meshed interface allows for easy application of discontinuities and interfacial physics.

Mesh is added and removed dynamically as the interface moves over time. This gives us the benefit of a level set method for handling topological changes with the power of a moving mesh method for handling discontinuities and jumps in material properties. Some drawbacks include mass loss similar to the underlying diffuse interface methods, evolving problem graph, file bloat and the expense of remeshing.

In previous work, CDFEM was developed for stationary fluid interfaces [1]. Extensions of the stationary approach to moving boundary problems proved to be a research effort on its own is discussed in a recent report [8] and a forthcoming paper [9].

The equations of motion, extent of reaction equations, and level set equations are discretized with the finite element method. A pressure stabilized Petrov-Galerkin method is used to reduce the condition number of the matrix, allow for equal order interpolation, and enable the use of Krylov-based iterative solvers [10]. Further details of the modeling approach and equations, the numerical methods used and the finite element implementation can be found in a paper Rao et al. [3]. It has been found that decoupling the problem into three matrix systems is the fastest approach to solving the problem. The momentum equations and continuity equation are solved as one system of equations, that require GMRES solve with ILUT fill factor 3. The energy equations and reactions equations are solved in a separate matrix and the level set method has its own matrix. The three matrices are loosely coupled and solved at each time step.

In Figure 3, we can see results from a CDFEM simulation of a Raleigh-Taylor instability. The inital condition shows a heavy green fluid over a lighter yellow fluid. The simulation maintains its symmetry to a great extent, and gives the result of a stable stratification of the yellow over the green fluid at long times, with very little mass loss.

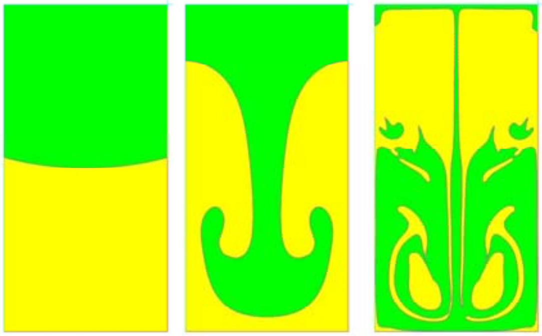

Figure 3. CDFEM algorithm is robust through entire Rayleigh-Taylor instability

The simulation is able to capture the both the coarse and fine features of this complex flow instability.

Results and Discussion

The mold and the finite element mesh for our validation efforts are shown in Figure 4. This is a good test case, since its complex geometry includes contractions, expansions, and a sinusoidal channel. In addition, there is a large section in the bottom of the mold that can have exotherms producing hot spots in the foam.

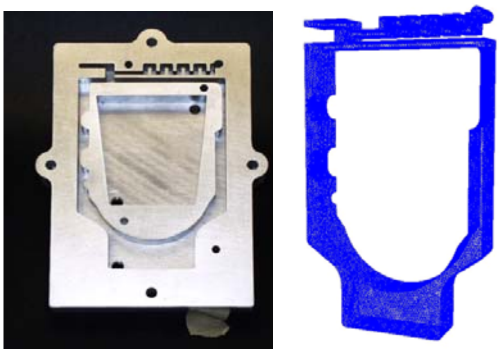

Figure 4. Kansas City mold (left) and finite element mesh (right).

We were able to fill a mold with PMDI-4 and record the images as seen in Figure 5. The corresponding finite element simulations can be compared to the flow visualization experiments and are also shown in Figure 5. From this figure, we can see that there is a good agreement between the model and the experiment.

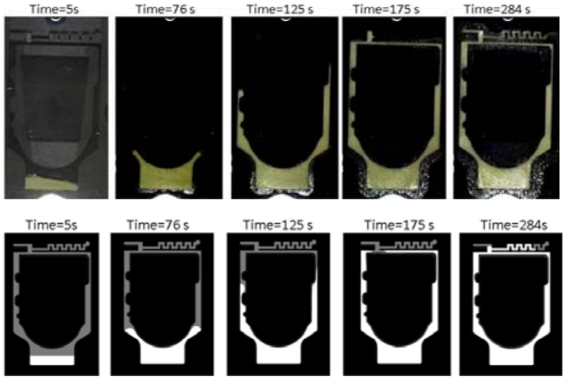

Figure 5. Flow visualization (top) compared to finite element simulations (bottom) for filling of the Kansas City Mold with PMDI-4.

Volume as a function of time can be seen in Figure 6. Here we can see that there is excellent quantitative agreement between the model and experiment. For this agreement to be possible, careful measurements had to be undertaken to determine the initial volume and density in the mold.

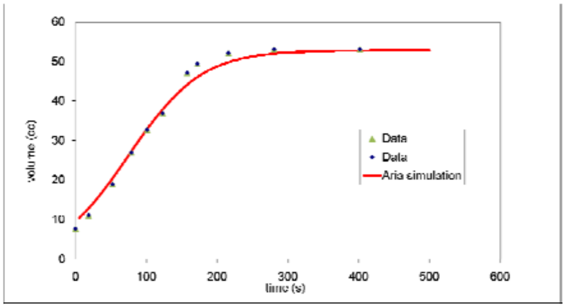

Figure 6. Volume as a function of time for finite element simulations and flow visualization experiments.

Once the PMDI-4 had polymerized and cooled down, it was possible to remove the sample from the mold. Because the foam adheres strongly to the mold, the top section of the mold with the sinusoidal flow feature did not release and was not included in the density analysis. Calibration samples were made of known density to determine the density of the part. Results from an X-Ray CT of the foam are shown in Figure 7.

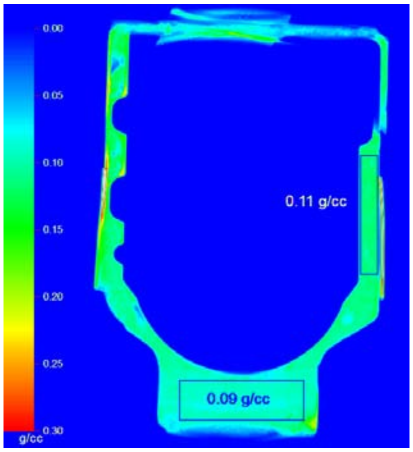

Figure 7. Experimental CT gives density gradients in the Kansas City Mold.

The density varies from 0.09 g/cc, at the bottom of the mold, to 0.11g/cc, in the center of the mold. High density regions of 0.30 g/cc can be seen near contractions in the mold. These are thought to be associated with bubble breakage due to high shear rates.

We can compare densities from our model to the experimental CT data. The results from this are shown in Figure 8.

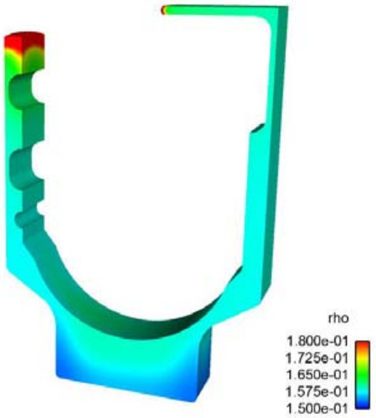

Figure 8. CDFEM model of extent of reaction for CO_2 generation gives correct trends of foam density variations. The foam density starts homogeneously at 0.95 g/cc and ends with a small gradient of 0.15 to 0.16 g/cc.

We initiate the model with a uniform foam density of 0.95 g/cc. In the final snap shot, it ends with a small gradient of 0.15g/cc at the bottom of the mold to 0.16 g/cc near the top of the mold. The experiments show at least an 18% variation in foam density. The simulations are only predicting a 7% variation in foam density, though this is an improvement over our previous model that predicted no density gradients [2, 3].

Conclusions

A new model has been developed to predict density gradients and final density in polyurethane foamed parts. The model couples the polymerization and foaming reactions to predict the degree of cure as the foam expands. A new numerical algorithm, CDFEM, has been used to determine the location of the foam-air interface over time.

The model is an improvement to the previous model (7% density variation vs .0%), but still has issues once the foam extent of reaction has reached completion. We are currently working to address these issues. New formulations are being tested, including a CDFEM implementation of the foam model that would allow a compressible gas phase.

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