Applications

Simulating Epoxy Curing with Exothermal Heat Effects

The exothermal curing process causes the material to self-heat, leading to internal temperature gradients. We simulate the curing of an epoxy in cylindrical aluminum containers with varying wall thicknesses (0.3 to 1 cm) under controlled thermal conditions: 120°C at the bottom, 100°C on the sides, and 25°C at the top. This simulation determines whether complete curing occurs throughout the volume after 130 minutes (figure 1).

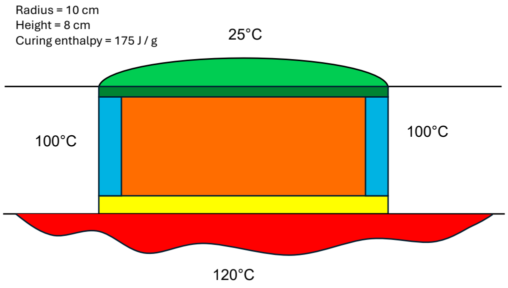

Figure 1: The simulation of curing is based on an aluminum container under the given conditions.

Simulation Results: Temperature Distribution

In figure 2, the simulation illustrates how temperature evolves over time along the vertical axis and radially at 66% of the cylinder's height. Due to the exothermal reaction, the material self-heats, resulting in a higher temperature at the center compared to the surrounding areas. At 130 min, temperature distributions are shown for both a vertical cross-section and a horizontal slice taken at 66% of the cylinder height, providing a clear view of thermal gradients during curing. The lower and central regions of the epoxy volume attain significantly elevated temperatures, whereas the top-center portion of the cylinder remains comparatively cool due to limited heat conduction and surface cooling (figure 3). The temperature plots reveal localized hot spots (red) resulting from the exothermal nature of the curing reaction. A prominent thermal peak is observed at approximately 4 cm in height and 6 cm radially from the cylinder wall, indicating a zone of intensified self-heating within the bulk material.

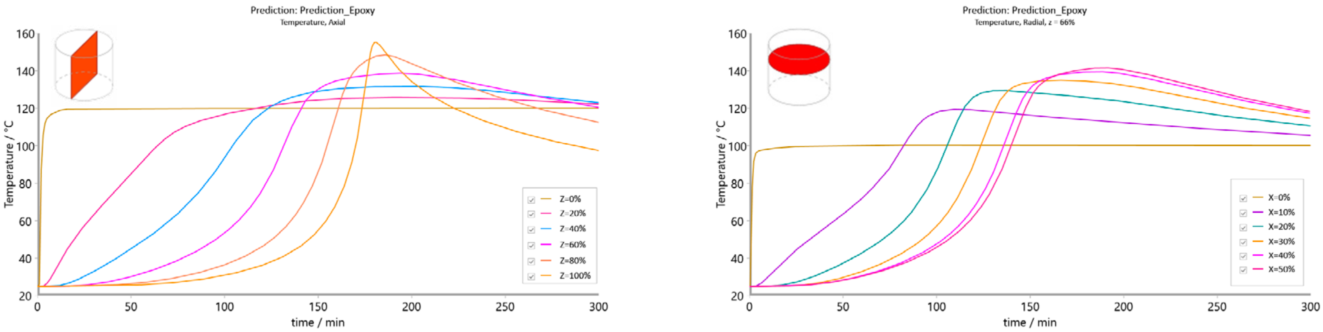

Figure 2: The simulation of the temperature in vertical and radial direction within the cylindrical container.

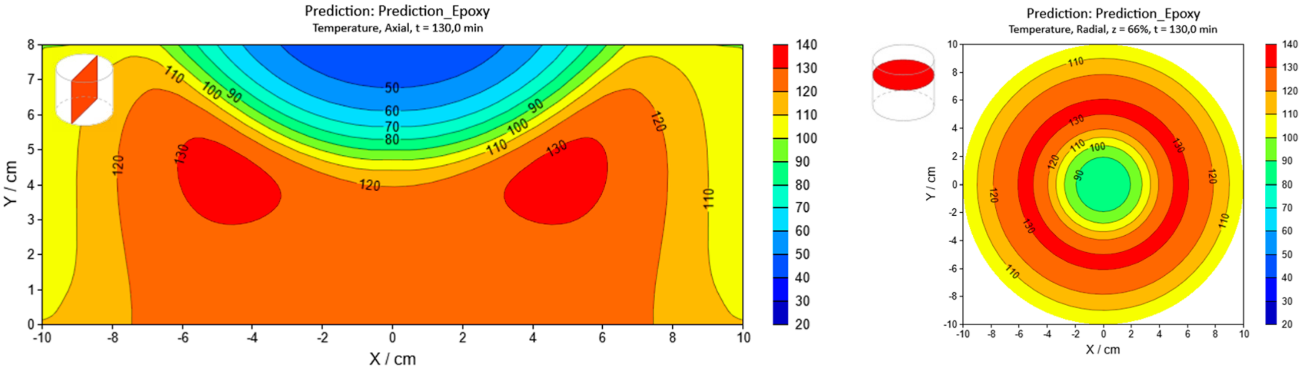

Figure 3: The temperature distribution of the vertical and horizontal sections in the cylinder at t=130 min.

Simulation Results: Conversion Rate

The distribution of the conversion rates is presented at a time of 130 min for both the vertical and horizontal cross-sections, with the data obtained at 66% of the cylinder's height (figure 4).

The reaction front propagates from the thermally heated bottom surface to the colder upper surface, driven by the thermal gradient. The regions indicated by red correspond to the highest observed reaction rates. The blue area, situated beneath the reaction front, signifies that the material has already undergone the curing process and the reaction has reached its completion. The blue area above the reaction front indicates that the material has not yet undergone the curing process

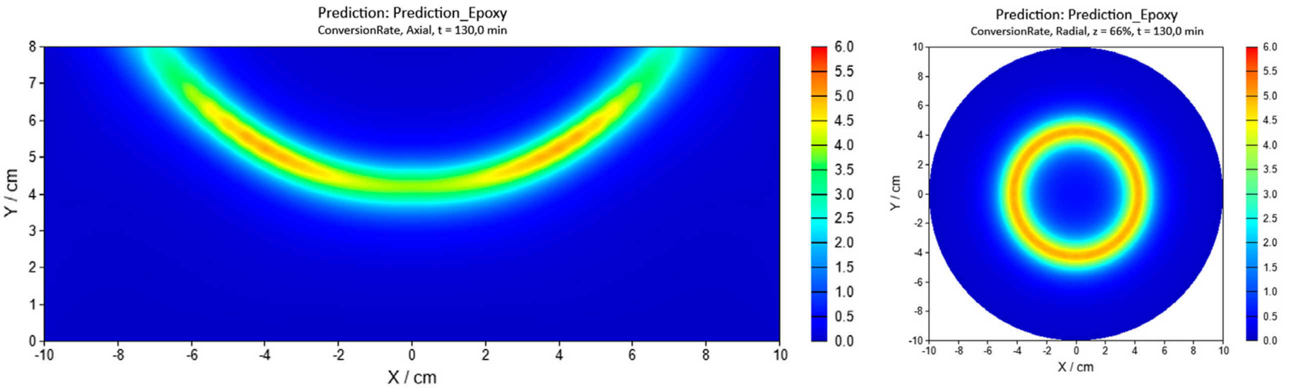

Figure 4: Simulation of the distribution of the conversion rate within the container.

Simulation Results: Degree of Conversion

Figure 5 indicates the degree of conversion for the horizontal cross-section at 50% of the sample height and a time of 130 min. The blue region in the center of the image indicates a low degree of cure near the vertical axis. The red regions, which indicate the maximum radius, signify completion of the curing process along the lateral surfaces.

The software facilitates the visualization of the cross-section at a user-selected vertical position within the cylinder.

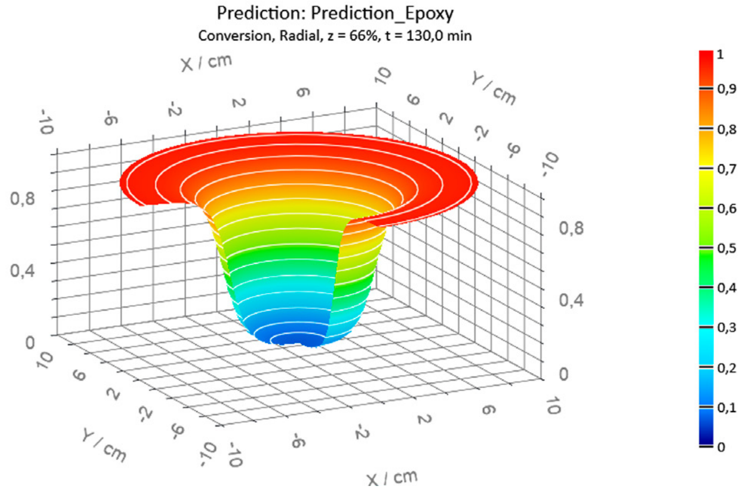

Figure 5: Simulation of the degree of conversion.

Glass Transition Temperature in the Curing Process

When a glass transition occurs during the cross-linking of a thermoset polymer, the reaction separates into domains dominated by different mechanisms. Far above the glass transition, the chemical reaction is fast and can be described by the Arrhenius relation. Near the glass transition, curing slows due to diffusion control. Below the glass transition temperature, the material vitrifies and the curing process slows down significantly.

This is why the kinetic model must be expanded with special diffusion control algorithms to account for the change in curing mechanisms.

Simulation Results: Temperature

The material temperature, T, which was measured at the 150-minute mark, was used to determine curing with diffusion control for both the radial and axial cross-sections (figure 1).

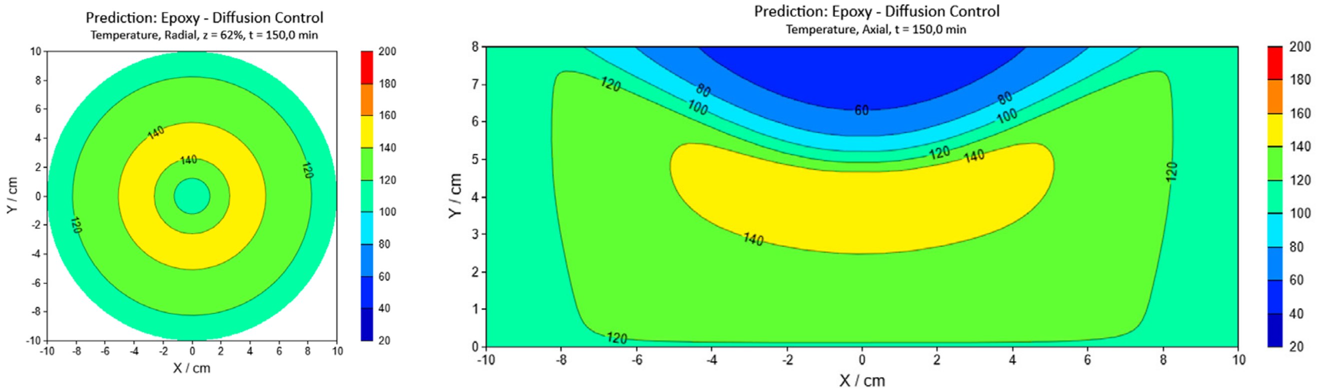

Figure 1: The simulation of the temperature at 150 min in radial and axial cross-section.

Simulation Results: Glass Transition Temperature

The prediction of the glass transition temperature (T_g) at 150 minutes is shown for both the radial and axial cross-sections, taking curing with diffusion control into account (figure 2).

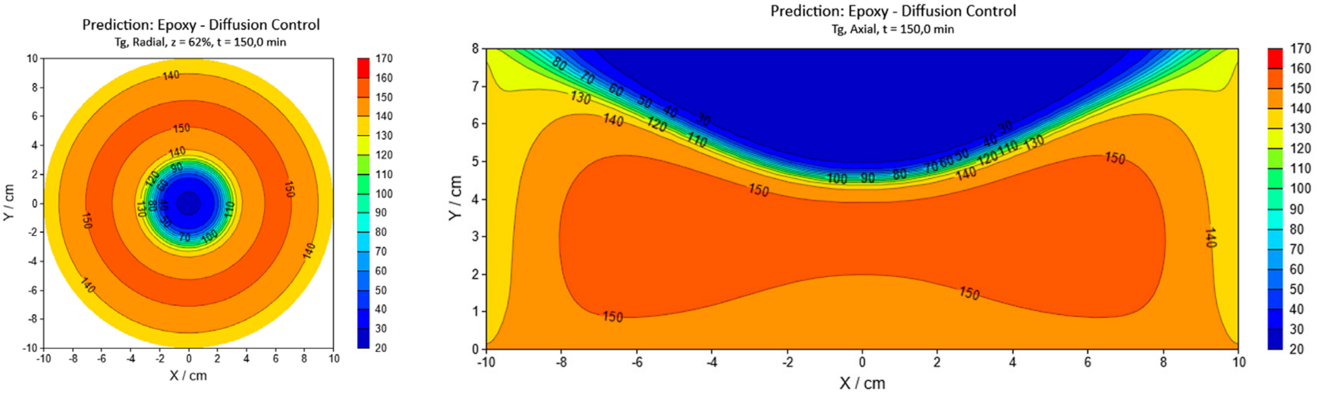

Figure 2: The simulation of the glass transition temperature.

If the current glass transition temperature, T_g, is below the current material temperature, then material is elastic/viscose, otherwise the material is vitrified and is in a glassy state.