

## **SIMULATION OF GLASS TRANSITION OF POLYSTYRENE**

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### **ABSTRACT**

The physical aging kinetics of polystyrene was utilized to simulate or predict the glass transition behavior of the polymer. The parameters that characterize the glass transition behavior are the glass transition  $T_g$ , Aging enthalpy  $\Delta H$ , Activation Enthalpy  $\Delta H_a$ , Cooling Rate  $R$  and Arrhenius Constant  $A$ . An experimented kinetic data of aged polystyrene was acquired from literature. The kinetic equations of polymer aging were manipulated to simulate the profiles of fictive temperature, heat capacity, heat flow and temperature change. The variation of these profiles on changes of cooling rate,  $R$ , non-linearity parameter  $X$  and distribution constant  $\beta$  were observed. Finally, these data were graphically analyzed and manipulated to acquire values of  $T_g$ ,  $\Delta H$  and also to back-calculate the aging constant:  $A$  and  $\Delta H_a$ . These calculated values were compared with experimented results in order to evaluate the feasibility of the simulation. These results and curve patterns matched that of the experimented data. It was also found that  $X$  and  $\beta$  impose little effect on  $T_g$  but influence a lot the thermal properties and rate of glass formation.  $R$  values on the other hand are influential on glass transition temperature. The results of the analysis suggested that the simulation is feasible in studying on physical aging and glass transition phenomenon of polymers.