

Concentrations for Multi-Step Processes

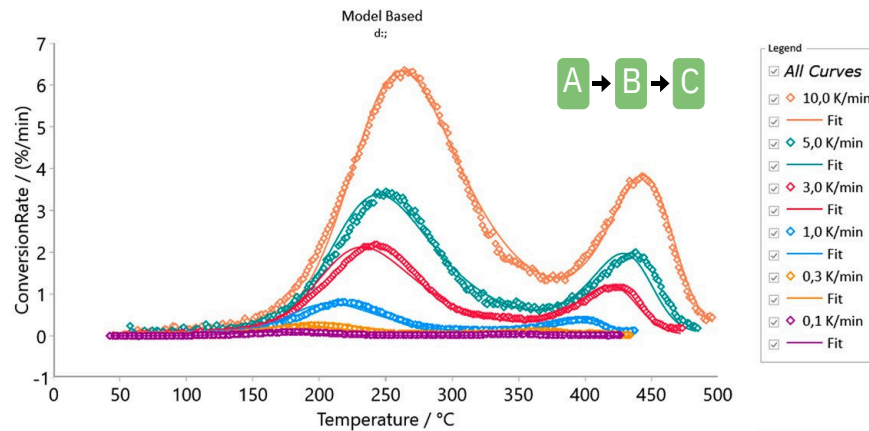


Figure 1. Kinetic model for a two-step decomposition process.

In multi-step reactions, the concentrations of intermediate and final reactants influence the mechanical and electrical properties of the final product. In order to achieve the homogeneous properties in the reacting volume, the distribution of all the reactant concentrations must be known. This example illustrates a two-step kinetic model $A \rightarrow B \rightarrow C$ with three reactants A, B and C (figure 1). Simulation of the two-step reaction in a cylindrical volume presents the

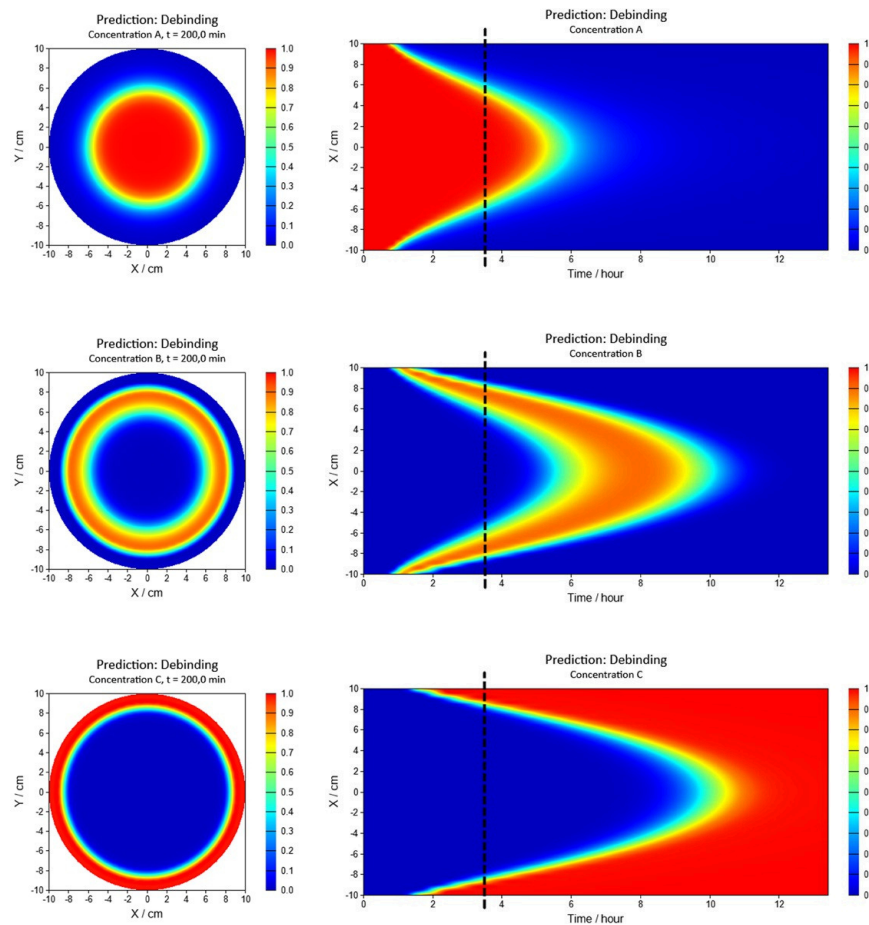


Figure 2: Prediction of the concentration levels of A, B, and C (left); and over time (right).

concentrations of all three reactants at selected time points. The rectangular plots in figure 2 show the time-dependent concentration at various radial points. The dashed line represents the time = 200 min, at which point the round cross-sections of cylinder are taken. Multi-step kinetic products contain

the initial reactant, the final product, and the intermediate reactants, which are important for some industrial applications.