# Unlocking the Differential Scanning Calorimetry Heat Signature

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This research delves into the realm of simulating reaction kinetics of materials using Differential Scanning Calorimetry (DSC). A mathematical model and a computational model have been developed to predict and analyze thermal characteristics on DSC curves, aiming to optimize machine-learning algorithms for kinetic parameter prediction. The study focuses on deriving theoretical models to generate simulated data due to the challenges of acquiring extensive real DSC data. By exploring various mathematical approaches, the research aims to characterize different reaction models through intricate analysis of the heat flow rate, reaction rate, and heat capacity variations in the sample. Emphasis is placed on formulating kinetic parameters, such as rate constants and activation energies, to model the degree of conversion during thermal events. Furthermore, the project introduces methodologies to preprocess DSC signals, including denoising techniques for signal accuracy. The investigation also includes fitting heat capacity variations of individual thermal events with the Shomate equation, enhancing the analytical capabilities of the software. Overall, this work lays the foundation for future advancements in predictive modeling and data analysis of DSC curves, paving the way for enhanced insights into material thermal behaviors and reaction dynamics.

**Keywords:** *Differential Scanning Calorimetry (DSC), simulation, analytical modeling, Shomate equation, signal denoising, reaction kinetics, heat capacity*