Sequential estimation of kinetic parameters for nutraceutical degradation using the Arrhenius model

Dharmendra K. Mishra[1], Kirk D. Dolan[1,2], JV Beck[3]

[1]Department of Biosystems and Agricultural Engineering
[2]Department of Food Science and Human Nutrition
[3]Department of Mechanical Engineering
Michigan State University, East Lansing, Michigan, USA

ABSTRACT

Diet and nutrition are increasingly linked with disease prevention and treatment. Nutraceutical compounds, such as anthocyanins, are food components known for their health promoting, disease preventing or medicinal properties. Nutraceuticals not only can act as bright natural colorants but also have potential health benefits, such as antioxidant and anti-inflammatory properties. Anthocyanin is one such nutraceutical present in grape pomace. The sequential estimation procedure was applied in this study to estimate the kinetic parameters for the degradation of anthocyanins in grape pomace. Sequential estimation is a diagnostic tool that can provide insight into the process of parameter estimation. It accounts for the each observation added to the estimation procedure and updates the parameters, thereby making it a dynamic estimation method for continuous processes. Grape pomace with moisture content of 42% (wb) was heated in steel cans (radius 0.027 m and height 0.073 m) in a retort at 126.7°C for times ranging from 8 to 25 minutes. Center temperature in canned grape pomace was measured during conduction heating, and was also predicted by the finite-element program. Thermal diffusivity was estimated using nonlinear regression by minimizing sum of squares of errors between the measured and predicted center temperature. Retention of anthocyanins in grape pomace was measured using high performance liquid chromatography. A first-order model with Arrhenius rate constant was used to predict the retention of anthocyanins. The Arrhenius parameters in the model were estimated using a nonlinear regression routine. The estimated values of rate constant, $k_{113.9^oC}$ and activation energy, E_a were 0.061 min^{-1} and 62.230 kJ/g mol respectively. The 95% asymptotic confidence intervals for $k_{113.9^oC}$ and E_a were [0.051, 0.071] and [17.40, 107.0] respectively. This method will help to reduce experimental effort and cost, as it can be shown that adding more observations will not necessarily change the parameter value after a certain time. These results indicate that the sequential estimation method can be used for optimal experimental design and determination of the adequacy of the model.