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Victoria Marsh* (vmarsh3@yahoo.com), Department of Mathematics and Statistics, 1250 Bellflower Blvd. - MS1403, Long Beach, CA 90840-1403, and Jen-Mei Chang and Stephen Mezyk. Numerical Methods for Optimizing Chemistry Kinetic Parameters.

The focus of this research is to find an analytic function representing experimental data by creating a computer program capable of optimizing the corresponding chemistry reaction kinetic parameters. The program will initially solve for the kinetic parameters of a specific reaction problem, a first order growth and second order decay reaction, simplified as $A \rightarrow B$, $2B \rightarrow C$. Using numerical analysis to generate an analytic function fitting the measured kinetic data, along with the differential equations corresponding to the reactions, an over-determined system of equations can be created. Using the measured reaction data values to solve this system of equations for the unknown kinetic parameters allows the program to calculate parameter estimations. By minimizing error, the program will then optimize the parameter estimators to best fit the experimental data. Preliminary results using a cubic spline approximation of the kinetic data, the program will optimize the corresponding kinetic parameters and allow for an analytic function to be created. The program will ultimately be expanded to handle more complex reaction systems. (Received September 22, 2011)