December 2016

Dear Reader,

This book was written in large part to assist with teaching a class on chemical kinetics for fossil fuel applications within the Department of Energy and Resource Engineering at Stanford University. The book is intended to teach general concepts, but the course goes further and involves calculations for applications that are too complex for a student to write their own computer codes. Exercises posted at this website use the computer codes Kinetics2015 and PMod2, which are also used in the class I teach. Partial answers are given for some exercises to help guide the student. New exercises will be posted at the beginning of each calendar year, along with the complete solutions to the exercises from the previous year. Comments and questions during the year are welcome.

Kinetics2015 is the latest version of a regression analysis program designed to extract global chemical kinetic parameters from multiple arbitrary thermal histories, written by Robert Braun and myself. The original application and largest group is in petroleum geochemistry, more specifically, deriving chemical kinetics that would reliably extrapolate from laboratory to geological time frames for petroleum exploration purposes. It has subsequently been used extensively for decomposition of minerals, polymers, biomass, and energetic materials. When initially developed in the mid-1980s, the user set up the problem via questions and answers in a DOS window. In the 1990s, it was converted to a Windows program. The current version is an enhanced version of the LLNL program licensed for commercial distribution to GeoIsoChem in 2009.

PMod2 is a chemical reaction simulator descended from but entirely different from PMOD, a Lawrence Livermore National Laboratory code written by Robert Braun and myself. Both were written with the objective of allowing the user to easily input any chemical reaction network into the simulator, which was actually a new concept back in the late 1980s when PMOD was originally developed. PMOD asked the user via a DOS window various elemental constraints on each reaction, and PMOD then calculated mass and molar stoichiometric factors from those constraints. It also did a single-phase EOS calculation for expulsion calculations in a compacting leaky reactor. PMod2 is simpler, with the user entering the chemical reactions with mass stoichiometric coefficients. The reaction progress can be calculated for closed and open systems, and geological expulsion is calculated using an extended Pepper-Corvi model. In the open system, the user can specify whether an oil species is volatile or non-volatile, and the former are immediately expelled from the reactor. The Pepper-Corvi expulsion model is basically a tank spill model in chemical engineering terms, where all species exceeding their sorption limit in the residual kerogen are immediately expelled from the reactor.

Both Kinetics2015 and PMod2 are available for purchase at the GeoIsoChem website (www. http://geoisochem.com/software/). Perpetual single-user licenses are available for both commercial and academic users, with the latter being half price. A new educational license for both codes has been established to aid the use of this book for classroom teaching. The educational license is an annual license for variable numbers of 6-month user licenses, with a half-price renewal fee each successive year.

Sincerely,

Alan Burnham