Mathematical modeling of oil shale pyrolysis

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The vast resource of oil shale in the United States can be transformed to a suitable alternative for transportation fuel. The knowledge necessary for the commercial implementation of a process to produce oil from oil shale is growing due to extensive research efforts. Technology has been proposed for commercial production in both in-situ and ex-situ modes to develop feasible process. During thermal pyrolysis, organic matter in oil shale decomposes and releases liquid (shale oil) and gaseous products. The decomposition process requires heat input. Several interrelated physical and chemical phenomena occur simultaneously, such as heat transfer, chemical reaction kinetics, multiphase flow, phase changes, and mineral alteration and interaction. Development of a complete model for these phenomena and the development of mechanistic pathways for the generation of products are required to optimize the effects of operational parameters. We are reporting the development of a computer model that simulates the product distribution that is constrained by elemental and product mass balances. A model in the COMSOL multi-phenomenon physics platform was developed that includes heat transfer due to conduction and convection, mass transport mechanisms, and phase equilibria. The secondary reactions of coking and cracking in the product phase were addressed and their formation kinetics were included. This general kinetic model was integrated with physical processes that occur during pyrolysis. The coupled governing equations were solved simultaneously and appropriate changes in physical properties of raw and product materials were taken into account as the decomposition process evolved. Experimental data from pyrolysis at different scales were used to validate the physical model. Parameter sensitivity analyses were conducted, and different cases were examined to optimize the process under different conditions. The comprehensive model developed in this study will help advance the commercial development of oil shale.