Global Chemical Kinetics of Fossil Fuels. How to Model Maturation and Pyrolysis
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Understanding of the chemical kinetics governing the transformation of fossil fuels has advanced tremendously over the past 50 years, but the diversity of fuel types, sub-disciplines, and applications has caused a lack of general understanding of how best to derive global chemical kinetic models for engineering and other modeling purposes. The first three chapters review the origin and structure of fossil fuels and advances in methods to derive global chemical kinetics of complex materials in general. The most appropriate type of global chemical kinetic model (e.g., autocatalytic, distributed reactivity) is related to the chemical structure of the fossil fuel. It then applies this knowledge to derive kinetic models that can be applied over a wide range of times, temperatures, pressures. Successive chapters consider these parameters in the context of various confinement conditions—open systems, semi-open systems, and closed systems. Applications are then presented for petroleum systems modeling (natural petroleum formation and migration), oil shale processing (in-situ and ex-situ), and coal pyrolysis, liquefaction, and combustion.