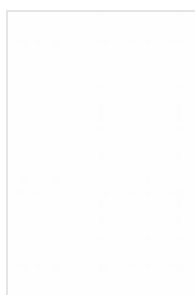


Developing Detailed Chemical Kinetic Models: Green Energy and Technology

With the increasing demand for clean and sustainable energy sources, the development of new and efficient technologies is essential. Chemical kinetic models play a critical role in the design and optimization of these technologies, as they provide a detailed understanding of the chemical reactions that occur during combustion and environmental processes.

This book provides a comprehensive overview of the development of detailed chemical kinetic models for combustion and environmental processes. The book offers a comprehensive discussion of the latest numerical and experimental techniques for kinetic modeling, including density functional theory, automated reaction discovery, and molecular dynamics simulations.



Cleaner Combustion: Developing Detailed Chemical Kinetic Models (Green Energy and Technology)

by Deane Montgomery

★★★★★ 5 out of 5

Language : English

File size : 13440 KB

Text-to-Speech : Enabled

Screen Reader : Supported

Enhanced typesetting : Enabled

Print length : 1040 pages

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Numerical Techniques for Kinetic Modeling

The development of detailed chemical kinetic models requires the use of advanced numerical techniques. These techniques can be divided into two broad categories: ab initio methods and semi-empirical methods.

Ab initio methods, such as density functional theory (DFT), are based on the fundamental laws of quantum mechanics. These methods can be used to calculate the potential energy surface of a chemical reaction, which can then be used to determine the reaction rate constants.

Semi-empirical methods, such as automated reaction discovery (ARD), are based on experimental data and empirical rules. These methods can be used to develop kinetic models that are less accurate than ab initio methods, but they are much faster and easier to use.

Experimental Techniques for Kinetic Modeling

In addition to numerical techniques, experimental techniques are also essential for the development of detailed chemical kinetic models. These techniques can be used to measure the reaction rate constants of individual reactions, as well as to validate the predictions of kinetic models.

Common experimental techniques for kinetic modeling include:

- Flow reactor experiments
- Shock tube experiments
- Laser-induced fluorescence experiments
- Molecular beam experiments

Applications of Chemical Kinetic Models

Detailed chemical kinetic models have a wide range of applications in green energy and technology. These applications include:

- The design and optimization of combustion engines
- The development of new and efficient fuels
- The design of air pollution control systems
- The study of climate change

This book provides a comprehensive overview of the development of detailed chemical kinetic models for combustion and environmental processes. The book offers a comprehensive discussion of the latest numerical and experimental techniques for kinetic modeling, as well as a wide range of applications of kinetic models in green energy and technology.



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