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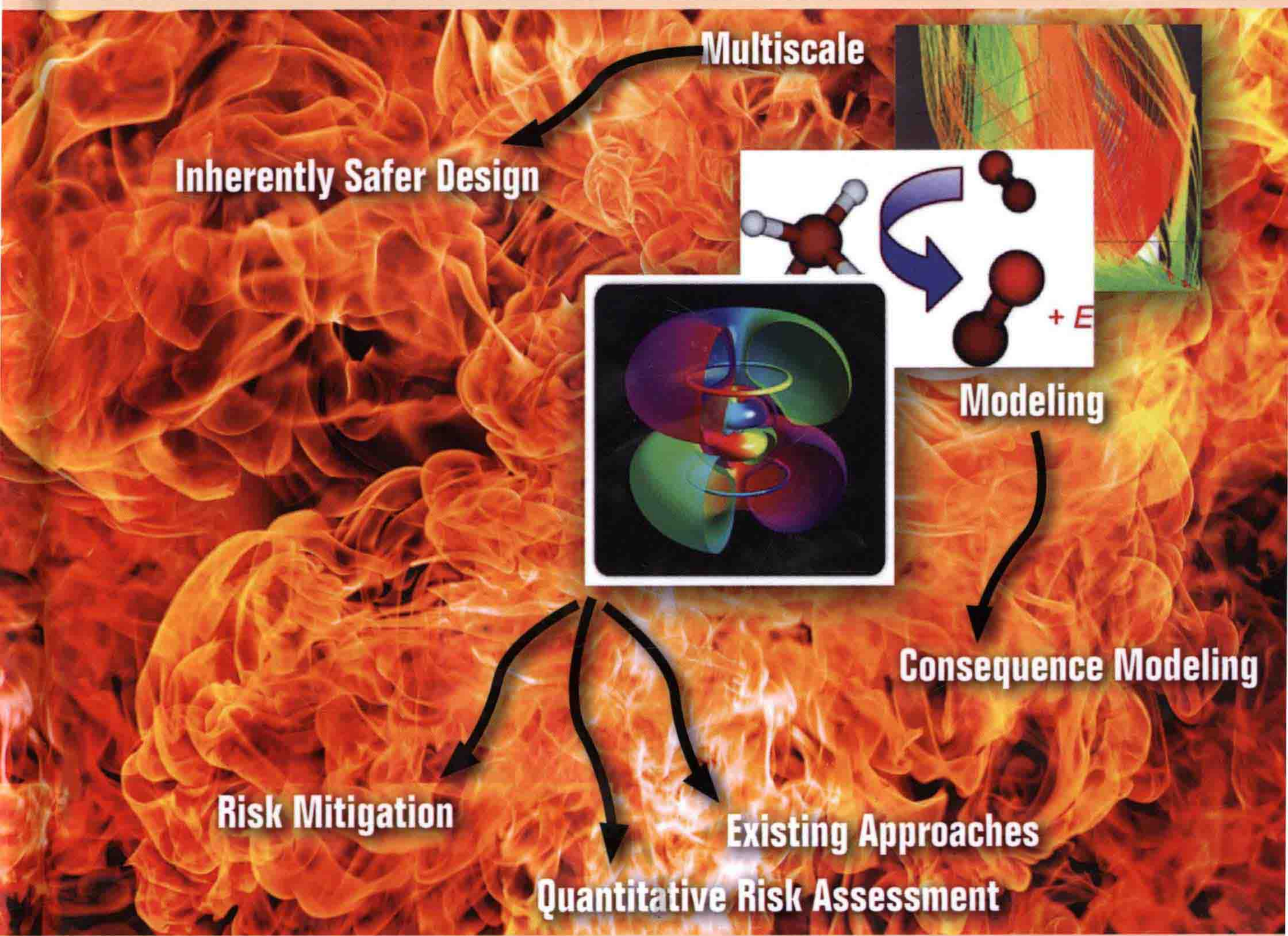
Multiscale Modeling for Process Safety Applications



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Preface

Computational modeling has emerged as a powerful partner to experimental and theoretical studies. It is a familiar subject in several fields but has so far been considered of secondary importance in process safety applications, which mostly relies on plant personnel experience and accumulated learning of the community from historical incidences. The current standard practices in assessment of hazardous scenarios or relevant parameters can be significantly aided by the wider implementation of detailed computational methods, at various time and length scales. Execution of these approaches, as explored in this book, has become more practical owing to the significant increase in computational power and ease of access to appropriate computational tools. Researchers across the globe have worked in exploiting these methods for process safety applications, but until now, the ensemble of these efforts has remained mostly as isolated studies. The main objective of this book is to group these existing efforts under a common platform by providing the current status of this novel area and discussing the potential implementation of multiscale modeling approaches for process safety applications.

Professionals, in both industry and academia, can use this book, as can graduate researchers working in any domain where process safety challenges are implicitly or explicitly embedded. To address such challenges, the book has attempted to cover applications of quantum mechanics, molecular dynamics, quantitative structure–property relationship, quantitative structure–activity relationship, computational fluid dynamics, finite element analysis, chaos theory, statistical analysis, and dynamic simulation as applicable. The problems dealt with are consequence modeling, risk assessment, and related parameter estimation for potential hazards resulting from fire, explosion, and dispersion of toxic gasses.

In this book, the bridge between various modeling methodologies is not discussed. In that sense, the individual chapters are essentially independent. Nor is the mathematical background of these multiscale modeling approaches discussed in detail. Fortunately, for each of these topics, several good books are available on the market. These sources can be used to supplement one's training in mathematical fundamentals.

Typically, problems at the level of quantum mechanics and molecular dynamics have dealt with safety-related concerns for a specific molecular system. At the molecular modeling level, it is more about material characterization in a given environment. Limited by time and length scale, these methods are not suitable for answering safety concerns for the whole process domain. However, knowledge gained at these scales, such as estimation of parameters at the molecular scale, can be passed on to a modeling environment with a lesser resolution for an atomistically informed holistic model. Another example of using two different scales in modeling approaches for addressing the same concern could be the use of a conservative low-resolution model for screening analysis and then the performance of detailed modeling of selected scenarios, similar to the Pareto principle.

Emerging tools and increasing computational power modeling in process safety have improved much from the case of a spherical cow, a metaphor used for highly simplified scientific models of complex physical phenomena. Accordingly, the use of detailed computational modeling approaches in combination with accumulated knowledge of safety experts can only contribute in a positive manner toward improving the safety performance of chemical facilities. This book is written with the hope that it will contribute toward promoting the use of multiscale modeling methodologies in addressing process safety problems.

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CHAPTER

INTRODUCTION

1

Concern for man himself and his safety must always form the chief interest of all technical endeavors. Never forget this in the midst of your diagrams and equations.
Albert Einstein

Numerous incidents such as the Flixborough explosion resulting from the release of flammable hydrocarbons in June 1974, the methyl isocyanate release in Bhopal in December 1984, and the Macondo disaster in 2010 continue to remind us of the important role of process safety in the design and operations of process facilities. Over the years, process safety has emerged as a discipline in itself and has continued to play a dominant role in any process technological development. While a focus on process safety model development, experiments at various scales have gained momentum over the years and had a positive impact on the industry, the safety incident databases are anything but stagnant (MARSH, 2014). Even recently, in August 2013, in response to recent catastrophic chemical facility incidents in the United States, President Obama issued an executive order to enhance the safety and security of chemical facilities, and consequently reduce the risks associated with hazardous chemicals, for owners, operators, workers, and communities.

Given the complexity of existing and emerging technologies, interactions of process parameters, and intangible and hidden correlations, quantitatively defining the underlying root of a process safety phenomenon, or predicting the same scenario, requires a great deal of experience, extensive knowledge, and a structured approach. Additionally, while experimentally quantifying process safety parameters is often insightful, it is resource intensive and often not comprehensive owing to the number of experiments that would be required to achieve the same. Experimentally validated multiscale modeling methodologies are powerful tools that have the potential to offer answers which are otherwise often expensive or unreachable through experiments. For example, think about large-scale jet fires or deflagration-to-detonation events. Typical current practice in modeling process safety scenarios is to substitute the lack of understanding by introducing conservativeness to a safety model. Unfortunately, conservative safety parameters not only increase plant costs, but may not ensure the safety of a facility. The insufficient details or coarser resolution of the solution has the potential to offer more risk than is mitigated by adding conservativeness to it. As we have demonstrated in a later chapter, mixtures exhibiting minimum flash point behaviors pose such a risk, and therefore exercising conservativeness alone may not be sufficient.

With significant rise of computational power in recent times along with better understanding of the underlying physics, implementation of higher-resolution models in order to gain insights and refine existing models to assess hazardous scenarios has become more practical and achievable. Owing to the multiscale nature of processes, multiscale modeling has emerged as a new set of tools that provides insight into important features at multiple times and lengths of a physical phenomenon. Thus, in several applications, it has become crucial to incorporate information from a range of length and time scales into a model (Cameron and Gani, 2011). As an outcome of modeling product and process issues, a growing number of modeling efforts are resulting in multiscale modeling approaches. The strategies discussed throughout the book, albeit in the context of process safety, attempt to capture inherently important properties at various scales of a system and correlate them accurately to the system's macroscale properties. A reasonable amount of work has been done in that respect in other areas, as demonstrated in several publications (Lépinoux, 2000; Kwon et al., 2007; Derosa and Cagin, 2010; Maekawa et al., 2008). Multiscale modeling techniques have been successfully employed in material design to rationally develop and accurately predict the performance of systems with the building blocks of their macroscopic-level performance residing at much smaller scales. Similar to other fields, it is only appropriate to extend the advancement in materials theory at different time and length scales to address less understood safety concerns by incorporating an adequate level of detail. In the context of process safety, while some sporadic work exists to assess problems at different time and length scales, to date those have been mostly isolated efforts. The primary objective in this book is to group these existing efforts on a common platform. This book aims to provide a review of the current status in this area, discuss potential implementation of multiscale modeling, and help refine existing computational approaches used for safety analysis. It attempts to provide an overall picture of how safety issues are addressed at all scales of modeling, and discusses the latest methods in the field.

Chapter 2 serves as the introduction to process safety. It touches upon the status of current industrially accepted state-of-the-art modeling approaches in process safety analysis. As appropriate, the chapter introduces or reintroduces the reader to process safety fundamentals such as the physics, consequences, and risks of fire, explosion, and toxic hazards in process industries. Concepts of flammability, ignition phenomena, fire, dispersion of flammable and toxic gases, deflagration and detonation, risk assessment of fire, toxic, and explosion hazards, are also covered in this chapter.

Chapters 3–6 deal with the use of modeling methodologies as applicable to process safety applications within various time and length scales. Chapter 3 demonstrates the applicability, relevance, and benefits of molecular modeling methods such as quantum mechanics, molecular dynamics, quantitative structure–property relationship (QSPR), and quantitative structure–activity relationship (QSAR) in process safety applications at various capacities. Chapter 4 moves into greater time and length scales and examines the effectiveness and benefits of implementing computational fluid dynamics (CFD) in the development of consequence models of process facilities. It looks into use of CFD in assessing the consequence of various types of fires such as jet, pool, and flash fires. It also looks at the modeling of explosion and blast waves using CFD. In a similar fashion, Chapter 5 illustrates the practicality of using finite element methods in process safety applications. Finite element methods have been implemented in understanding flare systems, storage and transportation of flammable materials, and other concerns in process hazard analysis. Accessing larger time and length scales phenomena are demonstrated through implementation of dynamic process simulations in Chapter 6. The transient nature of a process is typically crucial in modeling plant start-up and shutdown phenomena. In the same chapter, chaos theory and statistical analysis are introduced within the context of addressing process safety concerns. Chaos theory can be applied to investigate runaway reactions and has the potential to provide early warning detection of same. Statistical analysis has been utilized to monitor real-time plant data. Multivariate statistical analysis can be applied to plant data that can in turn help in incident investigation.