Control of Polymerization Reactors

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To our wives, Linda (FJS), Meena (PBD), and Debby (KWL),
to our students and teachers, and to Dr. Daniel E. Burke
of Exxon Chemical Company, Baytown, Texas

Preface

The field of synthetic polymers has grown tremendously over the last several decades. Today, polymers are found in a large variety of products—e.g., automobiles, paints, and clothing, to name a few. Polymers have replaced metals in many instances, and with the development of polymer alloys, applications in specialty areas are certain to grow. The new and highly specialized application of polymers, along with the trend toward total quality management and global competitiveness, has served to drive up the quality expectations of the customer. These developments make it imperative to operate the polymerization processes efficiently, which underscores the importance of optimizing controls.

The motivation for this text is the current paucity of books that deal with automatic control of polymerization reactors. An important feature of this work is that it offers the combined treatment of the principles of polymerization reaction engineering *and* the automatic control concepts for polymerization reactors. It is intended to serve as a text for an advanced undergraduate or graduate level course in the chemical engineering curriculum. Instructors should find the text particularly useful because it offers a combined treatment of the steady-state and control aspects of polymerization processes; it is often difficult to accommodate two or more different courses in any one specialty, such as polymerization, into the graduate curriculum. The book should also serve as a valuable reference for engineers in industry.

The first four chapters are concerned with the fundamentals of polymerization kinetics and reactors; the rest of the book is devoted to the study of control strategies for batch and continuous polymerization reactors.

We begin in Chapter 1 with a very brief review of the principles of polymer science. Here we introduce the concept of macromolecules and molecular weights of polymers, followed by a discussion of property–structure correlations of thermoplastics and thermosetting polymers and a description of the methods for analyzing the various properties of polymers. We follow this with a discussion of the chemistry and kinetics of various polymerization reactions. The list includes step-growth polymerization, free radical polymerization, anionic polymerization, and cationic polymerization.

Chapter 2 is devoted to mathematical modeling of polymerization reactors, and the kinetic analysis of anionic, free radical, and step-growth homopolymerization and copolymerization reactions. Chapter 3 deals with polymerization reaction engineering. In this chapter, we study the selection of the type of reactor for the manufacture of a selected polymer; batch, semibatch, continuous stirred tank, and plug flow reactors are considered. We presume a background appropriate to the engineer who has had a single undergraduate course in reactor design. Chapter 4 is devoted to heterogenous polymerization. Here, the processes and kinetics of suspension polymerization, emulsion polymerization, and coordination polymerization are covered.

The first four chapters contain many examples that illustrate the concepts. Chapters 2, 3, and 4 form an introduction to polymerization reaction engineering. Whereas their brevity makes them a less than perfect text from which to teach a complete course in polymerization reaction engineering, they are included for a number of reasons. First, we expect the background of the readers to be varied. Even those who have had a course in polymer science may not have had much exposure to polymerization reaction engineering. Second, we wish to use these chapters to lay the groundwork in the unique features of polymerization reactors that result in unique control problems. Finally, because much of the material in the later chapters involves model-based control, it is important to understand the techniques of mathematical modeling, the basis of such models of polymerization systems, and their relative merits. Certainly a full course in polymerization reaction engineering would be beneficial to the person wishing to work in polymerization control, but this text will introduce that subject when a dedicated course is not available.

With the material presented in the first four chapters, one can design a polymerization reactor and specify operating conditions. To operate the reactor, however, an understanding of control concepts would be required. The rest of the book is devoted to the study of control concepts relating to polymerization reactors. It is assumed that the reader has had a course in basic control systems concepts and is familiar with sampled data control concepts.

In a polymerization reactor, raw materials are mixed at specified operating conditions to produce polymer(s) having desired properties. The end-use properties of interest include color, viscoelasticity, thermal properties, and mechanical properties among others. To produce a polymer with such desired properties means that process variables such as temperature, molecular weight, molecular weight distribution, and Mooney viscosity must be tightly controlled. The manipulated variables available for controlling the variables of interest at setpoints include the flow rates of raw materials and catalysts, temperature of feed streams and temperature, and/or flow rates of heating/cooling mediums.

Automatic control of polymerization reactors is complicated for the following reasons:

Polymerization processes are highly nonlinear; the use of linear controllers often results in poor performance.

Many polymerization systems are open-loop unstable; therefore safety considerations are of paramount importance.

Polymerization reactor control systems are multivariable in nature. Process interactions, deadtime, and constraints complicate the control systems design of these units.

Many of the important variables such as molecular weight, molecular weight distribution, and Mooney viscosity cannot be measured directly. They must be inferred from other measurements. Inferential measurements can lead to erroneous results and, therefore, automatic control systems that are based on such measurements must be designed to accommodate such errors.

We describe the methods that are available to tackle these and related problems.

In Chapter 5, we describe the polymerization reactor control problem and identify the important end-use properties, controlled variables, manipulated variables, and disturbance variables. Chapter 6 describes the methods for the measurement of important process variables. Methods for estimating those variables that cannot be measured directly are also covered. Next, we describe methods for obtaining a dynamic model of the polymerization reactor. In Chapter 8 we show that in some cases single-input single-output (SISO) strategies can be effectively used for control. Included in this chapter are a number of modern approaches for SISO control. Chapter 9 is concerned with multivariable control strategies for polymerization reactors. Multivariable control must be used where SISO systems and multiloop control do not give adequate performance. In Chapter 10, we describe the nonlinear control techniques that may be applied to polymerization reactors. Chapter 11 is an introduction to polymer processing and to how product properties determined during the polymerization may affect processing. Throughout the second part of the text, the concepts are reinforced by examples and applications.

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Contents

1

Introduction to Polymerization

In this chapter the fundamentals of polymerization as they apply to control of polymerization reactors will be highlighted. Section 1.1 will give a very brief overview of polymeric structure. Sections 1.2 through 1.5 will present the four basic mechanisms of polymerization; a fundamental knowledge of polymer science will be presumed. For a good treatment of the subject, the reader may refer to the texts by Billmeyer [1], Rodriguez [2], Rudin [3], Williams [4] and Odian [5]. Structure–property relationships are well covered by Seymour and Carraher [6].

1.1 Macromolecules

This section will provide a starting point for the discussion of polymerization reactions and their control. The section is broken into three major topics: a brief description of polymer structures, a systematic definition of the molecular weight distribution (MWD), and a brief description of techniques of polymer analysis. An overview of polymer structures is included to motivate later discussions of control of polymer structure. The description of MWD serves to define the nomenclature for later use. The discussion of polymer analysis is meant to lead into later applications of on-line measurements of polymer properties. Recent advances in polymer characterization can be found in Ref. [7].