25–30 ft in diameter and have a five-to-one length-to-diameter ratio. High linear velocities serve to fluidize the catalyst particles that form; fluidization facilitates removing the heat of reaction. Catalyst is added continuously and polymer particles are removed once they reach a particular size (about 500–1000 μm). The reactor diameter is larger at the top, which lowers the linear velocity and acts to disengage the polymer particles from the unreacted gases. These same reactors are used for LLDPE. The choice of catalyst and the presence of inert gases and comonomers are used to regulate the polymer resin properties and molecular weight. The reactor typically operates at 220–370 psig and 160–205°F.

1.4.4 Hepatitis B Virus Modeling

As a final example, we wish to display the wide scope of chemical reaction modeling principles. Consider Figure 1.16, which shows some of the biochemical reaction events that occur in a single cell during the reproduction cycle of the hepatitis B virus [4, p.767]. The understanding and modeling of these biochemical events is an area of current research activity [14, 20, 21, 16].

The following is a simplified but useful model of part of this reproductive system

$$\text{nucleotides} \xrightarrow{\text{cccDNA}} \text{rcDNA} \tag{1.1}$$

$$\text{nucleotides} + \text{rcDNA} \longrightarrow \text{cccDNA} \tag{1.2}$$

$$\text{amino acids} \xrightarrow{\text{cccDNA}} \text{envelope} \tag{1.3}$$

$$\text{cccDNA} \longrightarrow \text{degraded} \tag{1.4}$$

$$\text{envelope} \longrightarrow \text{secreted or degraded} \tag{1.5}$$

$$\text{rcDNA} + \text{envelope} \longrightarrow \text{secreted virus} \tag{1.6}$$

These reactions correspond to the following steps in Figure 1.16:

1. Reaction 1.1 accounts for Steps 5, 9–11.
2. Reaction 1.2 accounts for Step 12.
3. Reaction 1.3 accounts for Steps 5–7.
4. Reactions 1.4 and 1.5 are not present in Figure 1.16, but may prove useful to explain potential loss of active cccDNA.
5. Reaction 1.6 accounts for Steps 13–15.

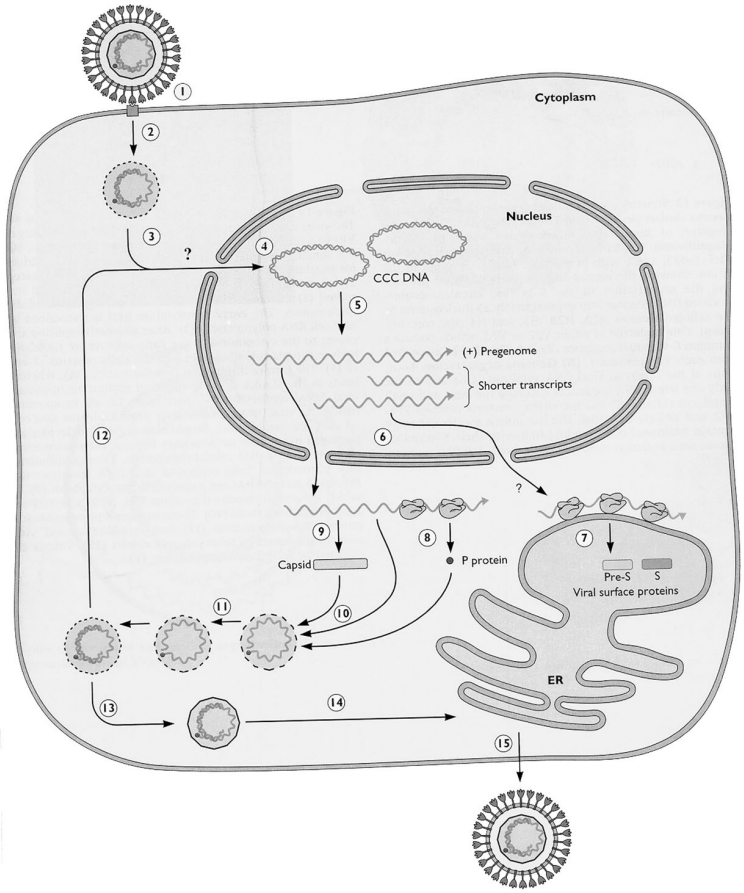

Figure 1.16: The chemical events comprising the reproduction cycle of the hepatitis B virus. Courtesy of ASM Press [4].

When we change to this context, the "chemical reactor" of interest becomes the living cell or, if we also model the cell population, the human liver. The chemical reaction modeling principles remain valid. In Chapter 4 we use this simple model to make quantitative predictions about the evolution of the viral species concentrations. We also show how to model systems that have small concentrations of species, down to less than a few hundred molecules. In Chapter 9 we explore estimating the rate constants that appear in this virus model given the kinds of laboratory measurements that are available.

Tailoring a model to make successful quantitative predictions of a system of interest is still more of an art than a science. We should not underestimate the complexity of some of the systems of interest to chemical engineers. Because we cannot include all the details, our models are always incomplete, and it is possible to make naive use of modeling approaches, and produce models with little connection to reality and little predictive value. This caution is perhaps especially true for biological systems. On the other hand, if we wish to increase our understanding of a chemically reacting system, skillful model building is often an indispensable part of the overall investigation. Simple models often can explain complex system behavior, especially when feedback mechanisms or autocatalytic steps are involved. The main goal of this text is to build the skill set with which chemical engineers apply reaction modeling tools to understand chemically reacting systems.

1.5 An Overview of the Text

Chapter 2. The remaining text is divided into eight chapters. We begin in Chapter 2 by discussing stoichiometry or the quantitative relationship between the different chemical species undergoing chemical reaction. We define chemical reaction rate and species production rate, and develop the accounting system for tracking the change in the reaction extent and the species concentration. Since most processes involve multiple chemical reactions, we make free use of matrices and linear algebra to summarize compactly the reaction stoichiometry.

Chapter 3. Next, in Chapter 3, we briefly review the important facts concerning the equilibrium state of a system undergoing chemical reaction. Most chemical processes do not reach equilibrium, but knowledge of the equilibrium state of the system allows one to define limits of reactor performance and identify operating conditions to realize desired production rates. The conditions for equilibrium are developed using the Gibbs energy and the chemical potential or species activity. We also briefly review phase equilibrium so that we are prepared for multi-phase reactions. The condition for chemical and phase equilibrium is generally stated as the minimization of an appropriate energy function or maximization of entropy. The use of numerical optimization methods is illustrated for solving complex reaction equilibrium problems involving many reactions.

Chapter 4. In Chapter 4 we develop the material balances for the three reactor types: batch (and semi-batch), continuous-stirred-tank,

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