

# Chapter 4: Entropy & Free Energy in Real Systems

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## Abstract

In this chapter, the authors have dedicated their time to the phenomenon of entropy and Gibbs free energy as the most important tools of quantifying the spontaneity and possibility of chemical reactions. The parameter known as entropy, which is used to measure the disorder of a system helps in determining in which direction a chemical reaction will take place and Gibbs free energy is relied upon to combine the enthalpy and entropy parameters in determining whether or not a chemical reaction is going to occur at a constant temperature and pressure. The chapter looks at the relation between the equilibrium constant and the free energy that presents an insight into the equilibrium in a reaction as well as in chemical thermodynamics. Their application in the industry e.g. in chemical synthesis, metallurgical processes, pharmaceutical production and energy storage are explained to justify the practical value of these concepts. Gibbs free energy knowledge helps chemists and engineers to select the most favorable conditions of a reaction, attain high yield, and develop processes that consume less energy. The chapter relates the theoretical thermodynamics with the actual use of free energy and entropy in an optimization and designing of processes in industries and developing sustainable processes of chemicals. This chapter has included a theory and practical examples in the modern industries and therefore provided a guideline that can be applied by students in carrying out scholarly research and in the industry to apply the concepts of thermodynamics.

**Keywords:** Entropy, Gibbs free energy, Spontaneity, Equilibrium constant, Industrial reactions, Thermodynamics.

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## 4.1. Introduction

Entropy and free energy are two essential thermodynamic parameters, which define the direction, feasibility as well as efficiency of the chemical processes within the real systems. Entropy, which is the measure of the molecular disorder, and free energy (and more particularly the Gibbs free energy,  $\Delta G$ ), which is enthalpy plus entropy, are also used to establish whether a reaction should occur spontaneously in applied chemistry. The real industrial systems are not idealized as compared to idealized models, and they commonly work at high pressures, non-ideal mixtures, impurities, and variable temperatures. Such conditions lead to deviations of ideal behaviour and therefore entropy variations and free-energy computations are necessary in the design of processes. In refinery processes, polymer production, food production, and pharmaceutical production, the knowledge of entropy is used to improve mixing, phase transition, and separation methods. Free-energy criteria are used to select catalysts, equilibrium in a reaction, and run a reactor at a lower energy expense. One of the applications of  $\Delta G$  is the viability of large-scale reactions, including ammonia synthesis, cracking, fermentation, and battery systems that are dependent on  $\Delta G$ . Also, the analysis of entropy generation is applied to determine the loss of energy and enhance sustainability. Therefore, entropy and free energy present a complete system, which can be used to maximize efficiency, safety, and productivity in actual industrial conditions. Enthalpy changes, entropy and Gibbs free energy ( $G$ ) are also used to identify spontaneity and equilibrium of reactions in chemical and industrial systems.

## 4.2. Gibbs Free Energy ( $G$ ) and Spontaneity

The Gibbs free energy ( $G$ ) is an important thermodynamic operation that is applied to predict the feasibility and direction of a chemical reaction at constant temperature and constant pressure, as is characteristic to most industrial processes. It is a combination of enthalpy ( $\Delta H$ ) and entropy ( $\Delta S$ ) and the equation is  $\Delta G = \Delta H -$