CHAPTER I

INTRODUCTION

Styrene is one of the most important members of a series of unsaturated aromatic monomers. Styrene is used extensively for the manufacture of plastics, including crystalline polystyrene, rubber-modified impact polystyrene, acrylonitrile-butadiene-styrene terpolymer(ABS), styrene-acrylonitrile copolymer(SAN) and styrene-butadiene rubber(SBR). Many different techniques have been investigated for the manufacture of styrene. More than 90% of the worldwide capacity to produce styrene is based on catalytic dehydrogenation of ethylbenzene.

The problems encountered in the ethylbenzene dehydrogenation in conventional reactors, as well as the possible solutions, are similar to those met in the dehydrogenation of alkanes. The main problems in the actual ethylbenzene dehydrogenation process are:

1. low conversion : due to thermodynamic limitations(equilibrium conversion around 40% at 900 K under atmospheric pressure);
2. high endothermicity of the reaction $\left(\Delta H^{\circ}_{298} = 28.1\text{kcal}/\text{mol}\right)$.

During the past decade, the concept of membrane reactor has been intensively investigated for a variety of different reactions. A membrane reactor combines a reaction with a separation process in a single unit. A major advantage of membrane reactor operation is that a conversion beyond its equilibrium value can be achieved by continuous removal of one or more reaction products using a membrane as shown in Figure1.1. The dehydrogenation of ethylbenzene to styrene is one of the reactions of interest in this type of applications. Improvement in membrane reactor performance can be obtained when using a membrane with high H_2 permeability and permselectivity for removing the product H_2 and, consequently the reaction mixture does not reach the equilibrium and the production of styrene should increase.

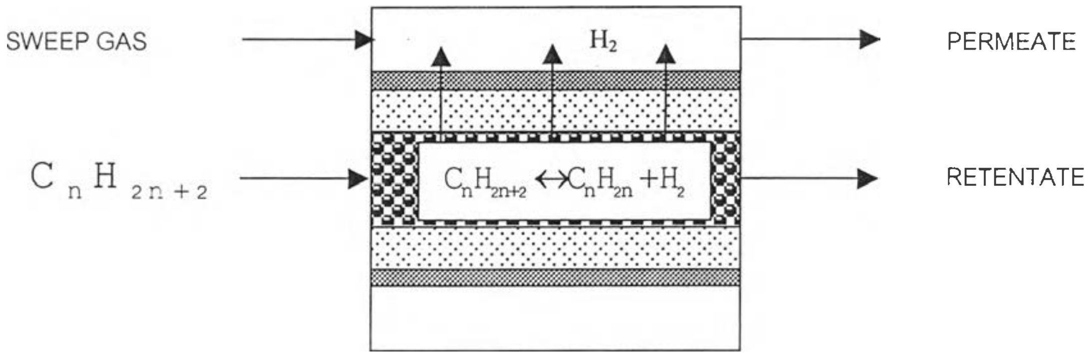

Figure1.1 Membrane reactor concept for dehydrogenation reaction.

There are various types of membranes employed for high temperature dehydrogenation reactions such as dense metal membranes (e.g. Pd or Pd-alloys), porous membranes (e.g. alumina, titania, zirconia, or vycor glass), and composite membranes (e.g. metal/alumina, metal/vycor glass, or metal/stainless steel). The most promising membrane for hydrogen separation nowadays is a palladium-based composite membrane because of high permeability and high permselectivity. The driving force for the removal of hydrogen form the catalyst bed is a gradient of the chemical potential between reaction and separation sides. Different options exist to establish this gradient, i.e. using vacuum, a pressure difference, inert sweep gas, or reactive sweep gas (i.e. air). All these methods decrease the partial pressure of hydrogen on the separation side to establish a hydrogen partial pressure gradient across the membrane.

Although a number of research has been carried out in the area including modeling of ethylbenzene dehydrogenation in membrane reactors, there is little effort in considering the effect of radial dispersion and non-isothermal condition. The objectives of this research are to use the two-dimensional mathematical simulation to investigate:

1) the effect of radial concentration and temperature profile;
2) the effect of operating parameters on the performance of a fixed-bed reactor and a palladium membrane reactor.