Modeling Hydrogen Spillover in Dual-Bed Catalytic Reactors

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DOI 10.1002/aic.10077

A semiquantitative model was developed to describe hydrogen spillover in dual-bed catalytic reactors. In previous studies it has been conclusively demonstrated that hydrogen can diffuse macroscopic distances and activate catalytic sites. The test reaction in those studies was the isomerization of 1-butene to 2-butene. The model is derived based on the fundamental principles of transport phenomena and reaction kinetics. Because many of the required values in the model are unknown, it cannot be solved quantitatively. Thus, a parametric analysis was conducted. The model successfully predicts trends observed experimentally. Specifically, the activity increases nonlinearly as the bed composition changes, the selectivity was low for all dual-bed reactors, and the selectivity was high for well-mixed catalyst beds. © 2004 American Institute of Chemical Engineers *AIChE J,* 50: 821–828, 2004

Keywords: spillover, dual catalyst bed, reactor analysis, mathematical modeling

Introduction

Traditionally, catalytic reactions are performed in reactors containing a homogeneous bed of a single catalyst. Recent work, however, demonstrates that combinations of catalysts can improve reactor performance, in terms of activity, selectivity, and deactivation (Chang, 1996, 1997; Weigle and Phillips, 2004; Delmon, 1993; Baumgarten and Meyer, 2000a). Phillips and coworkers described such a catalyst system for the isomerization of 1-butene to 2-butene (Chang, 1996, 1997). Their reactor contained a physical mixture of two catalysts: a noble metal (Pt, Pd) supported on graphitic carbon and a bimetallic containing a base metal (Fe, Co), and a Lanthanide metal (Ce, Pr) also supported on graphitic carbon. The activity of their beds increased as the amount of bimetallic catalyst in the reactor increased. This fact is significant because the bimetallic catalyst alone shows no hydrocarbon conversion at the temperatures employed. Furthermore, Weigle and Phillips (2004) demonstrated that the activity increase is maintained when the two catalysts are present as distinct zones within the reactor. In fact, the reactants can be fed such that 1-butene only contacts the bimetallic catalyst, yet substantial hydrocarbon conversion is measured. In all these cases, the activation of the bimetallic catalyst was attributed to atomic hydrogen diffusing from the noble metal surfaces to the bimetallic surfaces and activating them.

Numerous authors have demonstrated hydrogen spillover in systems where the hydrogen-generating surface is separated from a second type of active site (Weigle and Phillips, 2004; Chang et al., 1996; Chang and Phillips, 1997; Delmon, 1993; Baumgarten and Niemeyer, 2000; Baumgarten and Meyer, 2000a,b; Baumgarten and Maschke, 2000; Najafabadi et al., 2002; Roessner and Roland, 1996). Perhaps the most dramatic examples of this were given recently by Weigle and Phillips (2004), when they showed that hydrogen can diffuse to surfaces several centimeters from the source of the atomic hydrogen. This observation raises the question of how the phenomenon can be exploited in reactor design. Several benefits can be envisioned: improved activity and selectivity toward the desired reaction products, decreased poisoning of noble metal surfaces, and reduced catalyst costs.

Perhaps surprisingly, no mathematical models exist to describe dual catalytic reactors linked chemically through spillover species. Such a model could be used to assess new reactor

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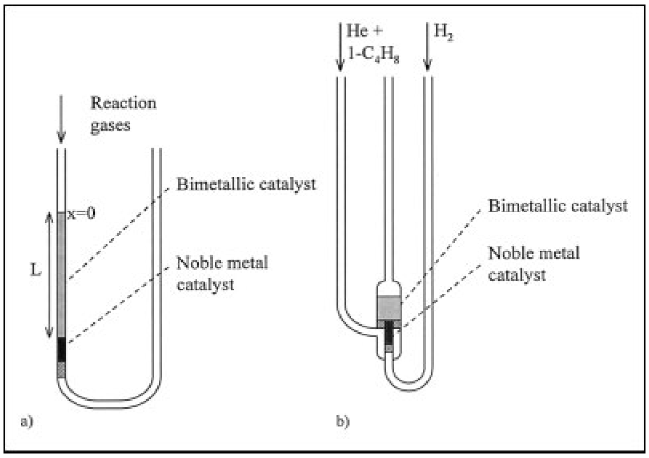

Figure 1. Test reactors: (a) dual-bed reactor, and (b) dual-bed, dual-feed reactor.

designs intended to exploit spillover. Although the model presented here cannot be used for final reactor design, even for the one reaction studied here due to a lack of detailed kinetic data, it can help broadly predict the relative efficacy of various designs, significantly reducing the scale of pilot plant efforts. The work can also be a template for models of other reactions or reactors in which spillover plays a significant role. Finally, the model suggests what data are necessary to understand spillover and to use it in improved reactor designs.

This work describes three semiquantitative models. Each model describes the selective isomerization of 1-butene in a reactor of unique geometry. The reactors have been described in detail previously (Chang and Phillips, 1996; Weigle and Phillips (2004). Each model contains the same kinetic expressions, but differ with respect to the transport and boundary conditions. Unfortunately, many of the constants are unknown, so quantitative predictions of the reactor performance cannot be made. However, the models were restated in parametric form, and reasonable estimates of the parameters were made. The models in parametric form were able to predict all of the trends observed in a dual-bed reactor, in a dual-bed dual-feed reactor, and in a reactor containing a homogeneous mixture of the two catalysts.

Experimental

The experiments that provide the data for comparison to the models are described in detail elsewhere (Chang and Phillips, 1996; Weigle and Phillips, 2004). In all the experiments, the catalysts used were a noble metal catalyst containing a noble metal, either Pt or Pd, supported on graphitic carbon, and a bimetallic catalyst containing a base metal, either Fe or Co, and a Lanthanide metal, either Ce or Pr, also supported on graphitic carbon. The first type of reactor contained a well-mixed bed of the two catalysts. The second reactor, referred to as the dual-bed reactor, was a simple U-tube containing distinct zones of the two catalysts, as seen in Figure 1a. The catalysts were in contact at the interface of the two zones, but they were not allowed to mix. The final reactor is referred to as the dual-bed dual-feed reactor, depicted in Figure 1b. Like the U-tube reactor, this reactor contained distinct zones of the two catalysts that were in contact at their interface. However, in this reactor, the feed material was introduced such that the noble metal was exposed only to hydrogen. After passing through the noble metal catalyst bed, hydrogen entered the bimetallic catalyst bed. The 1-butene was fed directly into the zone of bimetallic catalyst.

The procedure for measuring total activity and selectivity toward 2-butene formation was identical for all reactors. First, only noble metal catalyst was loaded into the bed. The catalyst was pretreated in flowing hydrogen at 300°C for 4 h, then the activity and selectivity were determined at temperatures ranging from 0 to 40°C. This test established the baseline activity and selectivity for the noble metal catalyst. The bimetallic catalyst was then added to the reactors in 10 – 30 mg increments. Except for the reactor containing the well-mixed bed (Chang and Phillips, 1996), the catalysts were not allowed to mix. The bed was re-reduced after each addition of the bimetallic catalyst, and the overall activity and selectivity were again measured.

Typical results for the U-tube reactor are shown in Figure 2a, and for the dual-bed dual-feed reactor in Figure 2b. For the U-tube reactor, the overall activity increased with each addition of bimetallic catalyst. However, the measured activity increase got smaller with each addition of bimetallic catalyst. The results were even more dramatic with the dual-bed dual-feed reactor. When only noble metal catalyst was present in the reactor (the point at 40 mg in Figure 2b), absolutely no 1-butene conversion was detected because the hydrocarbon never contacted the noble metal catalyst. The activity increased dramatically once bimetallic catalyst was added to the reactor. Since the bimetallic catalyst by itself has no activity at these temperatures, it was concluded that hydrogen spillover activated the bimetallic catalyst sites in the reactors.

Model Development

Unlike most catalytic systems with low conversion, the three reactors in this study cannot be modeled as differential. The experimental results show that different sections of the dual-bed reactors have significantly different behavior. In addition, the bimetallic section must be considered nondifferential because of the sharp atomic hydrogen gradient resulting from spillover. Thus, even though the conversion of 1-butene is low and its concentration can be considered constant throughout the reactor, the overall process cannot be modeled as a differential because of the varying hydrogen atom concentration within the reactor.

The model as presented in this development characterizes the U-tube reactor when the gas flows downward through the catalyst bed; that is, when the bimetallic catalyst is located upstream of the noble metal catalyst. The experimental results for this situation are given in Figure 2a. To begin modeling the phenomena leading to these results, it is necessary to understand the hydrogen dynamics within the reactor. The proposed steps involved in activating the bimetallic catalyst are shown in Figure 3. The first step in the process is the dissociative adsorption of molecular hydrogen onto the noble metal surface, forming atomic hydrogen. Because H_2 is fed in large excess, the hydrogen surface concentration can be considered constant, and in equilibrium with the gas-phase molecular hydrogen, over the length of the noble metal zone. The bimetallic catalyst cannot dissociate H_2 at these conditions, but atomic hydrogen

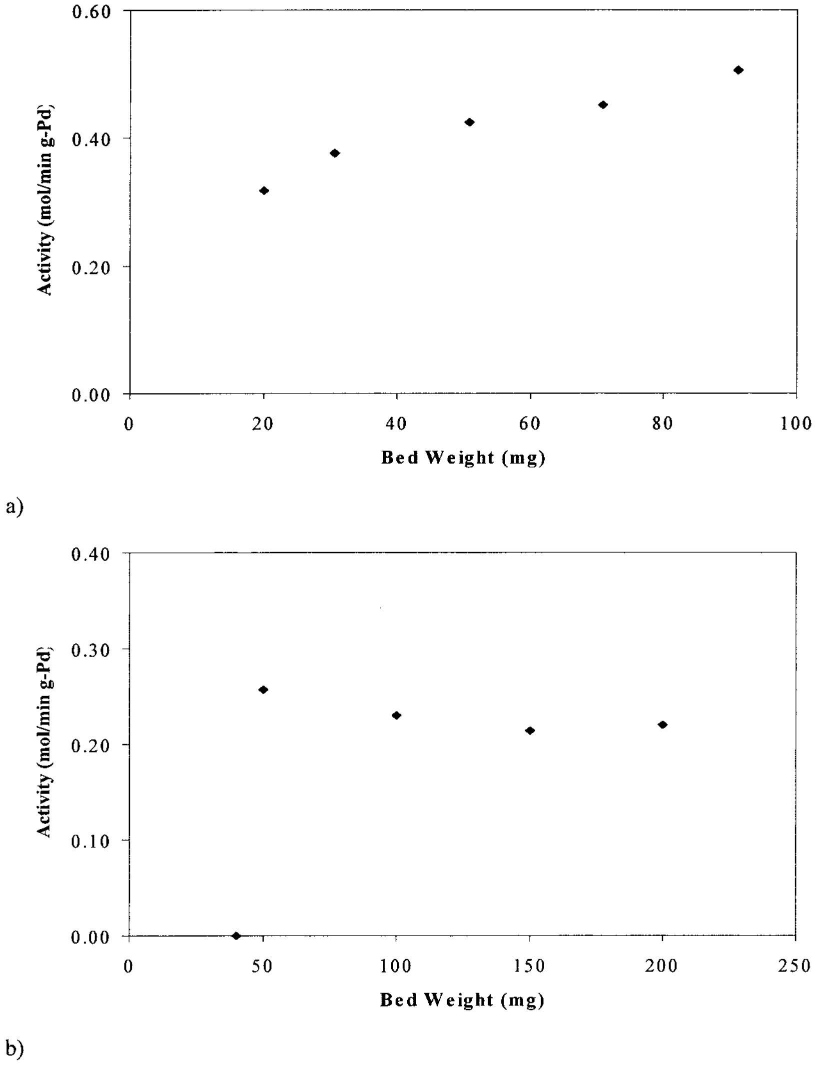

Figure 2. Experimental results for the dual bed reactors.

Activity changes as FeCe/Grafoil catalyst is added to Pd/Grafoil catalyst in the (a) U-tube reactor, 40°C, and (b) dual-bed, dual-feed reactor, 0°C.

can diffuse into the bimetallic catalyst zone. The surface hydrogen concentration over the bimetallic can only decrease by two mechanisms: recombination to form H_2 and reaction with butenes to form butane. This establishes a concentration gradient and "pumps" atomic hydrogen into the bimetallic zone via surface diffusion (hydrogen spillover). Once the bimetallic catalyst sites have been activated by atomic hydrogen, 1-butene from the gas phase can adsorb and react via the experimentally determined (isotope exchange) hydrogenation and isomerization mechanisms (Wells, 1967, MacNab and Webb, 1968; Mellor and Wells, 1969a,b; Burwell and Schrage, 1965) which involve only atomic, and not molecular, hydrogen.

Three irreversible reactions are considered for the reactor model: hydrogenation, isomerization (double bond shift), and hydrogen recombination. The assumption of irreversibility is justified since equilibrium strongly favors the reaction products (*cis*-2-butene, *trans*-2-butene, and butane). As explained below, the surface hydrogen concentration is not in equilibrium with the gas-phase hydrogen in the bimetallic section of the reactors; therefore, it is necessary to write the reactions in terms of surface hydrogen concentration. In the model, the hydrogenation rate is assumed proportional to the 1-butene partial pressure and the surface hydrogen concentration squared. These are reasonable assumptions since the reaction occurs between one adsorbed 1-butene molecule and two surface hydrogen atoms. In addition, experiments on hydrogenation kinetics over noble metals reveals that the reaction is approximately first-order with respect to the hydrogen partial pressure (Wells, 1967; MacNab and Webb, 1968; Mellor and Wells, 1969a,b; Burwell and Schrage, 1965), which corresponds to second-order with respect to dissociated hydrogen. The isomerization rate is considered first-order with respect to both 1-butene partial pressure and surface hydrogen concentration. Again this is reasonable since the surface reaction involves one 1-butene molecule and one hydrogen atom. Finally, hydrogen recombination is treated as second-order with respect to the surface hydrogen concentration.

The model characterizes the reactions within the bimetallic

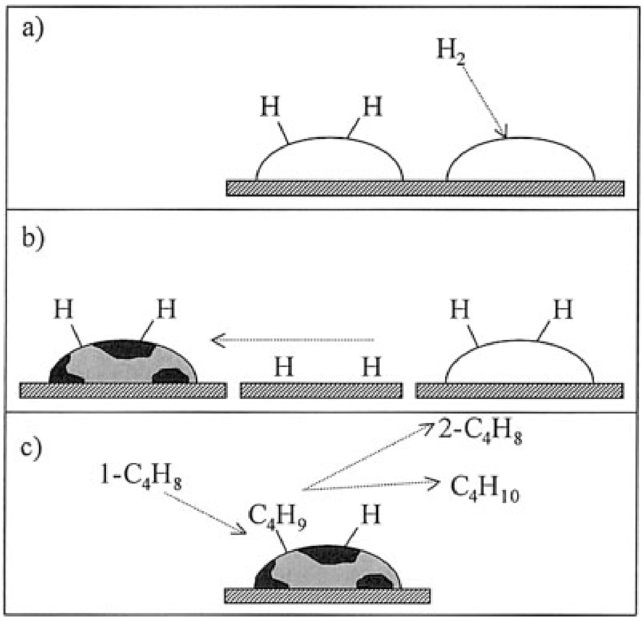

Figure 3. Hydrogen dynamics within the U-tube reactor.

(a) Molecular hydrogen adsorbs and dissociates over the noble metal catalyst (b) atomic hydrogen diffuses along the support surface to the bimetallic catalyst sites (c) 1-butene adsorbs and reacts at a bimetallic site, forming either 2-butene or butane.

zone of the reactor. The key equations are a 1-butene balance (1) and a surface hydrogen balance (2). The boundary conditions are chosen so that the partial pressure of 1-butene at the inlet to the bed, and the surface hydrogen concentration at the noble metal-bimetallic interface are fixed. The concentration gradient of atomic hydrogen at the inlet of the bed is zero. In other words, atomic hydrogen does not diffuse out of the bed. On the basis of the model assumptions outlined earlier, the differential mole balances are

$$0 = -\left(\frac{\dot{V}}{RT}\right)\frac{dP_{1B}}{dx} - \left(\frac{\pi D^2}{4}\right)(k_H P_{1B} C_{H,S}^2 + k_I P_{1B} C_{H,S}) \qquad (1)$$

$$0 = D_{H,S}\frac{d^2 C_{H,S}}{dx^2} - (k_R C_{H,S}^2 + 2k_H P_{1B} C_{H,S}^2) \qquad (2)$$

$$P_{1B}|_{x=0} = P_{1B}^0$$

$$C_{H,S}|_{x=L} = C_{H,S}^L$$

$$\left.\frac{dC_{H,S}}{dx}\right|_{x=0} = 0$$

The reaction rate terms in the above mole balances are written in a different form than rate laws for conventional catalytic reactions. Specifically, the hydrogen concentration is not expressed in terms of its partial pressure. Instead, the rate expressions are written in terms of the concentration of atomic hydrogen on the surface. This is equivalent to assuming that the surface concentration of atomic hydrogen is not in equilibrium with the gas phase. Typical catalytic mechanisms with surface reaction as the rate-limiting step assume the surface species concentrations are in equilibrium with the species' partial pressures. However, local equilibrium cannot be assumed when the mechanism involves spillover. The very definition of spillover is that the adsorbed species diffuse to a surface where they normally would not adsorb. Dissociated hydrogen is present on the bimetallic catalyst solely because of surface diffusion, and cannot be in equilibrium with the gas phase.

The primary problem with direct application of this model is that many of the physical and kinetic constants are unknown. However, a parametric analysis can be completed by converting the model to a dimensionless form. As discussed later, doing this allows the model to be evaluated with reasonable estimates of key parameters. The following variable substitutions are made.

$$\bar{P}_{1B} = \frac{P_{1B}}{P_{1B}^0}$$

$$\bar{C}_{H,S} = \frac{C_{H,S}}{C_{H,S}^L}$$

$$\bar{x} = \frac{x}{L}$$

Upon substituting the dimensionless variables, Eqs. 1 and 2 become

$$0 = \frac{d\bar{P}_{1B}}{d\bar{x}} + \left(\frac{Vk_I P_{1B}^0 C_{H,S}^L}{n_{1B}^0}\right)\left(\frac{k_H C_{H,S}^L}{k_I}\bar{C}_{H,S} + 1\right)\bar{P}_{1B}\bar{C}_{H,S} \qquad (3)$$

$$0 = \frac{d^2\bar{C}_{H,S}}{d\bar{x}^2} - \left(\frac{k_H P_{1B}^0 C_{H,S}^L L^2}{D_{H,S}}\right)\left(\frac{k_R}{k_H P_{1B}^0} + 2\bar{P}_{1B}\right)\bar{C}_{H,S}^2 \qquad (4)$$

and the boundary conditions become

$$\bar{P}_{1B}|_{\bar{x}=0} = 1$$

$$\bar{C}_{H,S}|_{\bar{x}=1} = 1$$

$$\left.\frac{d\bar{C}_{H,S}}{d\bar{x}}\right|_{\bar{x}=0} = 0$$

Physical significance can be assigned to each dimensionless group in the above equations. Parameter I, $Vk_I P_{1B}^0 C_{H,S}^L / n_{1B}^0$, represents the ratio of the maximum possible isomerization rate to the 1-butene feed rate. Parameter II, $k_H C_{H,S}^L / k_I$, is the ratio of the hydrogenation and isomerization reaction rates. Parameter III, $k_R / k_H P_{1B}^0$, is the ratio between the hydrogen recombination rate and the hydrogenation rate, and Parameter IV, $k_H P_{1B}^0 C_{H,S}^L L^2 / D_{H,S}$, is a type of Thiele modulus, the ratio of the hydrogenation rate to diffusion rate, for the reactor.

The advantage to using the dimensionless form of the model is that the first two parameters can be estimated based on the experimentally measured conversion and selectivity. Parameter I is set to be much larger than the measured conversions to 2-butene. That is, the measured isomerization rate to butene feed rate was 0.025. Thus, the maximum isomerization rate to butene feed rate is set in the model to be 0.15. The trends predicted by the model are relatively insensitive to large variations in this parameter, 0.05 to 0.2. Parameter II is set to be 5 based on the known selectivity (Lu et al., 1994) of the bimetallic catalyst, 80%, and an assumed low normalized surface hydrogen concentration 0.05. Reason indicates that the normalized surface hydrogen concentration must be significantly lower than its value on the noble metal, 1.0. However, the concentration of spillover hydrogen was simply assumed to be of the order of 5% of the concentration of the hydrogen atom source. The trends in the model were also relatively insensitive to physically reasonable values of this parameter.

The other two parameters could not be estimated from existing data. Parameter III is a ratio of unknown rates. Knowledge of the hydrogen recombination and hydrogenation kinetics is required to calculate Parameter III. Studies of olefin isomerization and hydrogenation (Wells, 1967; MacNab and Webb, 1968; Mellor and Wells, 1969a,b) have focused on noble metals as catalysts, and the kinetic parameters reported therein are not applicable to the bimetallic catalysts used in this study. Similarly, there are some studies of hydrogen recombination in the astrophysics literature (Biham et al., 2001; Pirronello et al., 1999) and in the plasma physics literature (Tanabe, 1997). However, these studies were conducted under vastly different conditions than those in the current experiments, and they cannot be readily extrapolated to yield appropriate kinetic constants. The lack of appropriate hydrogenation kinetics also prevents calculation of Parameter IV. Therefore, in the parametric study, Parameter III was set to 1 and Parameter IV was varied between 1 and 100.

The model development for the bimetallic section of the dual-bed dual-feed reactor is identical to that of the dual-bed reactor, except for the boundary conditions. In the dual-bed dual-feed reactor, 1-butene flows in the same direction as hydrogen surface diffusion. This difference changes the boundary conditions as follows

$$P_{1B}\big|_{x=L} = P_{1B}^{0}$$

$$C_{H,S}\big|_{x=L} = C_{H,S}^{L}$$

$$\left.\frac{dC_{H,S}}{dx}\right|_{x=0} = 0$$

The dedimensionalization is the same as before, as are the estimated values of the dimensionless parameters.

An equivalent model for the well-mixed beds studied earlier is produced by eliminating the transport equation for atomic hydrogen (Eq. 2) and establishing a constant atomic hydrogen concentration throughout the reactor. The appropriate value for the surface hydrogen concentration, in order to compare the model results to those of the dual-bed reactors, was established by calculating the average surface hydrogen concentration present in the dual-bed reactor. Mathematically,

$$\bar{C}_{H,\text{avg}} = \int_{0}^{1} \bar{C}_{H,S}\, d\bar{x}$$

where the concentration profile of surface hydrogen is determined from the dual-bed simulations.

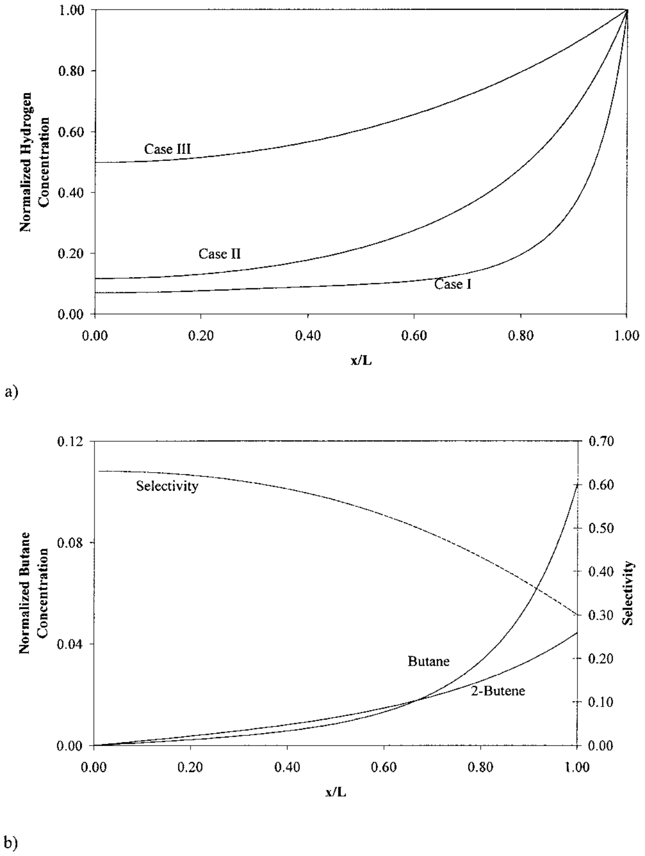

Figure 4. Model results for the dual-bed reactor, spillover is *countercurrent* to the bulk flow.

(a) Effect of the ratio of hydrogenation rate to surface diffusion rate; and (b) Product profiles through the bimetallic catalyst zone.

Model Results

Only the value of the hydrogenation rate to atomic hydrogen surface diffusion rate (Parameter IV) was varied during the simulations of the dual-bed reactor. Figure 4 summarizes the impact of varying the hydrogen surface diffusion rate through the bimetallic section of the dual bed reactors. Three cases are shown: high, intermediate, and low relative hydrogen atom diffusion rates. Case I represents the case where diffusion is low compared to the reaction rate (Parameter IV = 100). In this instance, very little hydrogen diffuses onto the bimetallic catalyst, thus, the hydrogen atom concentration throughout the bed is low, and the overall bed activity is low. Only 6.9% of the 1-butene is converted, and the selectivity to 2-butene is 36.7%.

Case III represents the situation where diffusion is rapid relative to the hydrogenation rate (Parameter IV = 1). In this case, the hydrogen atom concentration is relatively high throughout the bed and consequently the activity is very high, with 35.3% of the 1-butene being converted. Perhaps surprisingly, the selectivity is only 23.0%, much lower than what was found in Case I. This difference can be understood from Eq 3. The selectivity is the ratio between the isomerization rate (always normalized to the value 1), and the sum of the hydrogenation and isomerization rates. Both rates increase as the normalized surface hydrogen concentration increases, but the

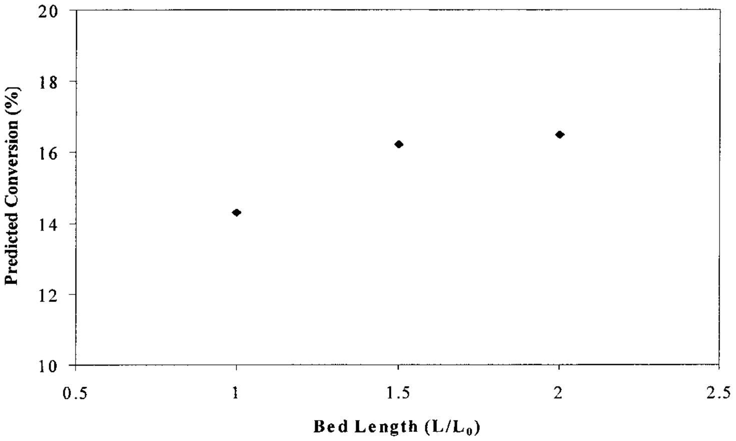

Figure 5. Effect of bed length on activity (Case II parameters).

As L increases, Parameter I increases in proportion to L and Parameter IV increases in proportion to L^2. Note the similar pattern between the model predictions and the experimental results in Figure 2a.

hydrogenation rate (second-order with respect to surface hydrogen) increases more quickly than the isomerization rate (first-order with respect to surface hydrogen). Thus, the selectivity decreases because increasing the relative diffusion rate increases the hydrogen atom concentration throughout the reactor.

Case II is believed to best represent the situation prevailing in the experimental studies. In this case, and intermediate value of the Thiele modulus was chosen (Parameter IV = 10). For this value of diffusion, high activity, 14.3% of the 1-butene feed converted, but still low selectivity compared to the pure bimetallic, only 30.1%, are predicted.

Figure 4b provides additional insight. For the intermediate diffusion case (Case II), it demonstrates how most of the reaction occurs in the portion of the bed with the highest atomic hydrogen concentration. About 50% of the reaction occurs in the 15% of the bed closest to the noble metal zone. Figure 4b also reveals a major selectivity shift as a function of position within the bed. The selectivity in the most active section of the bed, where hydrogen atom concentration is high, is very poor. In contrast, selectivity in the section of the bed with low hydrogen atom concentration is very high. This result suggests that high selectivity cannot be achieved in the dual-bed reactor since the section of the bed near the noble metal, the section where the majority of the reaction occurs, always contains a high atomic hydrogen concentration.

Figure 5 shows the impact of increasing the amount of bimetallic catalyst in the bed, based on the Case II parameters. As the bed length increases, Parameter I scales in proportion to L and Parameter IV scales in proportion to L^2. The simulation predicts that the conversion increases from 14.3% at $L/L_0=1.0$ to 16.5% at $L/L_0=2.0$. Most of the activity increase occurs when going from $L/L_0=1.0$ to $L/L_0=1.5$. While the absolute values of the conversions do not match experimental results, this trend is in complete agreement with the experimental observation (Figure 2a) that an activity plateau is achieved after a certain amount of catalyst is loaded into the reactor. The model predicts only a slight selectivity increase, from 30.1% at $L/L_0=1.0$ to 33.2% at $L/L_0=2.0$. This result is expected since the added catalyst is in a region of the reactor with low surface hydrogen concentration. Again, the same trend was observed experimentally.

The results are only slightly different when the dual-bed, dual-feed reactor is simulated. In this simulation, the same parameter values used in Case II above were used. The results are given in Figure 6, and they do not differ significantly from the Case II results below. The conversion was 15.1% and the selectivity was 30.0%. It might be expected that the conversion would be slightly higher, and the selectivity slightly lower in this scenario. These effects could result from the high 1-butene and high surface hydrogen concentrations occurring in the same portion of the bed. However, as can be seen by comparing Figures 4b and 6b, the majority of the reaction still occurs in the portion of the bimetallic zone closest to the hydrogen atom source, regardless of flow direction. This result is significant because it indicates that the noble metal catalyst can be completely removed from the hydrocarbon stream without sacrificing the activity of the bimetallic catalyst.

The simulation of a well-mixed catalyst bed was also made based on the Case II simulation of the dual-bed reactor. The average atomic hydrogen concentration (dimensionless) in the bed is 0.313. The predicted selectivity is much higher, 39.0%, if axial dispersion of hydrogen is neglected and instead the average hydrogen concentration is present throughout the reactor. The overall conversion is predicted to be 11.3%. Qualitatively, this agrees with the observations of Chang et al., 1996. For a well-mixed bed, they measured both higher activity and higher selectivity to 2-butene than in the U-tube reactor studies.

Given the great uncertainty in the values employed in the model, it is not reasonable to make quantitative comparisons between the model and experimental results. There is value in reiterating the finding that the model can predict trends that are consistent with those observed experimentally. Given realistic values for key parameters, the model reproduces the activity synergy, as well as the lack of significant selectivity synergy, found experimentally. Further work with the model is only appropriate if experimental values of the key parameters can be determined.

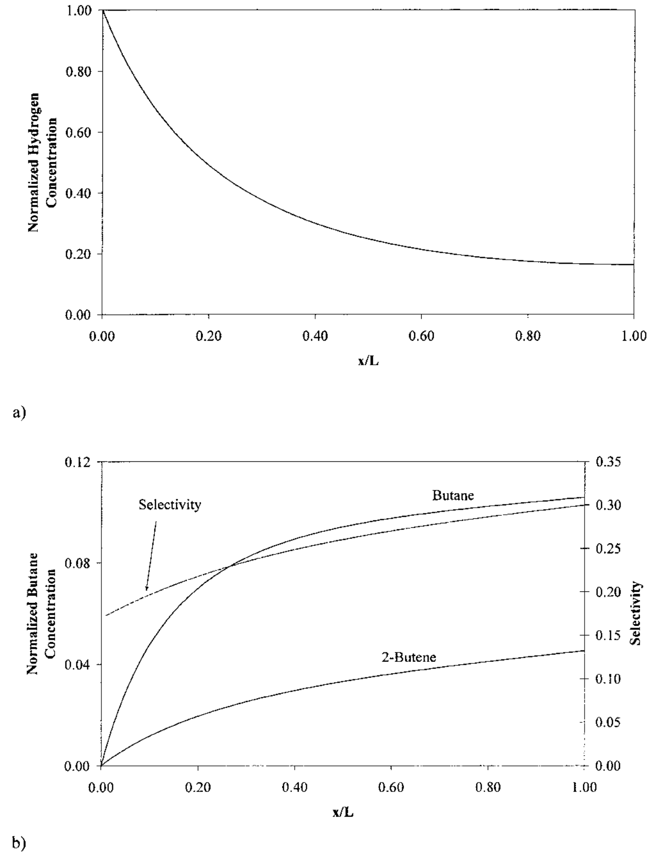

Figure 6. Model results for the dual-bed, dual-feed reactor, spillover and bulk flow are *cocurrent*.

(a) Hydrogen profile within the bimetallic catalyst zone; and (b) product profiles through the bimetallic catalyst zone.

Conclusions

The work described in this article represents the first attempt to incorporate hydrogen spillover via surface diffusion into the design equations for a catalytic reactor. Experimental work (Weigle and Phillips, 2004) conclusively demonstrated the ability of atomic hydrogen to diffuse macroscopic distances along graphitic surfaces. Diffusion occurred even when the concentration gradient of surface hydrogen was countercurrent to the bulk flow. The model developed in this work successfully reproduces the three significant observations from the experimental work. First, the presence of atomic hydrogen is necessary for 1-butene activity on the bimetallic catalyst. Second, as the diffusion length increases, that is, as more bimetallic catalyst is added to the reactor, the overall activity of the reactor increases, but at a decreasing rate. Finally, the selectivity toward 2-butene was always lower than when the reaction occurred over a well-mixed bed. This effect was due to the high atomic hydrogen concentrations near the interface between the bimetallic and noble metal catalyst zones. Also, it is important to realize that the consistency of the model with the experimental results does not *prove* that spillover is occurring. Rather, it demonstrates that all of the experimental observations are consistent with the spillover model, and all of the model predictions are consistent with the experimental trends.

Developing design equations that successfully incorporate spillover can be of great value. Potential benefits include higher activity, improved selectivity toward the desired products, inhibited catalyst deactivation, and lower catalyst costs. For these benefits to be realized, however, more study is needed. Many of the parameters for the model presented here remain unknown. More study is needed to determine appropriate values for the surface diffusion coefficient and rate constants. Once the true values of these constants are known, the model can be quantitatively compared to the experimental results.

Notation

$C_{H,S}$ = surface hydrogen concentration
$\bar{C}_{H,S}$ = dimensionless surface hydrogen concentration
$\bar{C}_{H,\text{avg}}$ = average dimensionless surface hydrogen concentration
$C^{L}_{H,S}$ = surface hydrogen concentration at the bimetallic-noble metal interface
D = diameter of reactor
$D_{H,S}$ = surface diffusion coefficient for atomic hydrogen
L = length of the bimetallic section of the reactor
k_H = rate constant for hydrogenation
k_I = rate constant for isomerization
k_R = rate constant for hydrogen recombination
n^{0}_{1B} = molar feed rate of 1-butene
P_{1B} = partial pressure of 1-butene
$\bar{P}_{1B}$ = dimensionless partial pressure of 1-butene
P^{0}_{1B} = partial pressure of 1-butene fed to the bimetallic catalyst
R = ideal gas constant
T = reactor temperature
V = volume of the reactor bed
$\dot{V}$ = volumetric flow rate of feed gas
x = length coordinate
$\bar{x}$ = dimensionless length coordinate

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Manuscript received Sept. 4, 2003, received Sept. 4, 2003, and final revision received Dec. 19, 2003.