An Experimentally Determined Configuration for Simulated Moving Beds as a Separative-Reactor in Gas Phase

S. Pakseresht¹, M. Kazemeini* and M.M. Akbarnejad¹

One of the most attractive features of Simulated Moving Beds (SMBs) is their ability to perform reaction and separation simultaneously in order to increase reaction yields. In this paper, an appropriate configuration for the operation of such systems in gas phase has been presented and to improve the separation efficiency, Pressure Swing Adsorption (PSA) is also employed. Fischer-Tropsch Synthesis (FTS) has been chosen to verify this idea. After preparing the catalyst, choosing appropriate adsorbent and constructing the necessary experimental set up, experiments have been performed to achieve maximum yield of desired products (i.e., ethylene and ethane). Effective variables, such as flow rates of the feed and carrier gas, ratio of reactants in the feed, switching time and the number of reaction and separation columns have been optimized empirically. The results of these experiments show that the combination of PSA and catalytic reaction causes an increase of product yields. Ultimately, experiments performed under optimized conditions demonstrated not only a reduction in consumption of CO by 10 percent but also indicated a rise in production of desired materials by the same amount. In addition, products are split into two extract and raffinate streams where the purity of desired C₂ products in the former stream is about 47 percent, which indeed is an improvement over most other previous techniques.

INTRODUCTION

Simulated Moving Bed (SMB) is an engineering innovation avoiding solid circulation difficulties in Moving Beds (MBs), such as channeling of the fluid stream, abrasion and attrition of the moving solid particles and fines removal from the system, while incorporating MB privileges. It is known that continuity and countercurrent increases the driving force and efficiency of mass transfer processes. Thus, MB has been introduced into the adsorption processes, where a solid phase (i.e., the adsorbent) moves countercurrent to the fluid phase in a continuous manner.

The countercurrent motion can be simulated by employing a fixed bed with several axially aligned inlets and outlets, moving the feed and product positions sequentially along them in the direction of the fluid flow. From the feed point of view, the fluid phase is moving forward while the solid phase is traveling backward. Alternatively, a configuration in which the fixed bed is replaced by a series of packed beds may be foreseen. In a multiple-column SMB, a port which can serve as inlet or outlet, is located between each column. Feed, desorber and product ports advancement in direction of the fluid flow simulates countercurrent motion in discrete steps at particular intervals. This is depicted in Figure 1. It is found that a multiple-column configuration of SMB is more convenient for laboratory investigation [1].

In binary separations, one component must be more strongly sorbed than the other. In true countercurrent flow, the strongly sorbed component convectively travels with the solid phase, while the weakly sorbed component is swept out of the system with the fluid phase. The column switching time (i.e., the time interval that a feed enters a column before it moves to the next column) is set between the breakthrough time of the two components. The weakly sorbed component elutes from the feed column before the feed is moved to the next column. The strongly sorbed

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product is retained in the feed column and is desorbed later. Countercurrent flow is simulated because the strongly sorbed component travels behind the moving feed point, while the weakly sorbed component moves ahead of it.

SMB can also be modified into different configurations to further improve productivity in accordance with specific applications. The number of beds or segments of a column is one of the effective parameters in optimal operation of these systems. On the other hand, it is possible to use more than one desorbent stream that adds yet another variable to evaluate the optimal configuration.

There is an SMB system that uses a single desorbent stream known as Sorbex family processes. These were developed by the UOP for petrochemical and sugar industries to facilitate liquid phase separations. The other class of separators uses multiple-desorbent streams. It is possible to use two or more desorbent streams for specific applications. In some difficult separations, use of multiple-desorbent streams helps to obtain products with higher purity. In these systems, each desorbent stream either elutes a product stream, or purges a column, thus, regenerating the adsorbent [2].

In reviewing the recent investigation of these systems, one can find some invaluable results. Ruthven et al. [3], Hashimoto et al. [4] and Barker and co-workers [5] pioneered the multiple-desorbent configuration, successfully separating mixtures which differ in equipment design. Some different section flow schemes have been evaluated by Tonkovich and Carr [2]. They compared advantages and disadvantages of them and concluded that each configuration may be proper for a particular separation.

On the other hand, SMB can also be used as a separative-reactor. A separative-reactor, initially known as a chromatographic reactor, is a device for carrying out chemical reaction and separation simultaneously in a fixed bed, filled by catalyst and adsorbent. It might not be a continuous process as a conventional fixed bed, since adsorbent should be regenerated. Therefore, an innovative application of SMB process involving a reactive mixture is termed a Simulated Moving Bed Reactor (SMBR). This is a novel reactor type in which separation occurs at the site of chemical reaction to improve product purity and conversion beyond those prescribed by thermodynamic equilibrium. When reaction and separation can be achieved simultaneously, the yield of the reversible reaction may be improved noticeably.

Through a simultaneous reaction and separation process, the purity of a multi-product reaction can be increased by separating out the products into two streams of extract and raffinate. Also, in this
phenomena, wastage of unreacted species is prevented while the reacting stream progresses to the next column in line.

Several investigations of SMBR have appeared in the open literature. A modified configuration of SMBR utilized for the Oxidative Coupling of Methane (OCM) reactions, has been recently employed by Tonkovich [6]. The other reaction investigated by Ray is the catalytic hydrogenation of mesitylene [7]. A conceptual evolution of SMBR is reviewed by Bjorkland and Carr [8]. Recently, Mazzotti [9] and Kawase et al. [10] have obtained good results in estrification reactions between organic acids and alcohols. In this work, ester and water were easily separated into high purity products. In Table 1 a list of major experimental work on SMBR available in the literature is sited in a compact manner.

In the present research, a new configuration of SMBR for a gas phase coupled with Pressure Swing Adsorption (PSA) to improve separation is introduced. For this purpose, Fisher-Tropsch synthesis is chosen for kinetic description of the system.

### NEW CONFIGURATION FOR SEPARATIVE- REACTOR WITH PRESSURE SWING IN GAS PHASE

Adsorbent regeneration is a vital step in every continuous adsorption process. Amongst different regeneration methods such as, temperature rising up, pressure decreasing and desorbent flow based upon the displacement technique, the latter one is very commonly utilized in SMB processes. However, pressure decreasing may also be combined together with desorbent flow in gas phase to improve regeneration process. Pressure increasing usually has a good effect on selective adsorption while pressure decreasing is a proper method for desorption step. However, one may use pressure swing desorption as an alternative.

<table>
<thead>
<tr>
<th>Research Subject</th>
<th>Researcher(s)</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Esterification reaction and separation in a SMBR</td>
<td>Sardin, Villermax (1979)</td>
<td>[12]</td>
</tr>
<tr>
<td>Glucose to fructose isomerization reaction in a SMBR</td>
<td>Hashimoto, et al. (1983)</td>
<td>[4]</td>
</tr>
<tr>
<td>Theoretical and experimental evaluation of a MB</td>
<td>Petroulas, et al. (1985)</td>
<td>[14]</td>
</tr>
<tr>
<td>Simultaneous reaction and separation for an equilibrium reaction in a MB</td>
<td>Fish, et al. (1986)</td>
<td>[15]</td>
</tr>
<tr>
<td>SMBR development as an enzyme reactor</td>
<td>Barker, et al. (1987)</td>
<td>[16]</td>
</tr>
<tr>
<td>Comparison between MB and SMB as chromatographic reactors</td>
<td>Fish, et al. (1988)</td>
<td>[17]</td>
</tr>
<tr>
<td>Experimental evaluation of reversible reactions in a MB</td>
<td>Fish, Carr (1989)</td>
<td>[18]</td>
</tr>
<tr>
<td>Different configurations evaluation of SMB as a chromatographic reactor</td>
<td>Ray, et al. (1990)</td>
<td>[19]</td>
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<tr>
<td>A few configurations for SMBR evaluation as a chromatographic reactor and separator</td>
<td>Tonkovich (1992)</td>
<td>[6]</td>
</tr>
<tr>
<td>Using SMBR as a chromatographic reactor and separator</td>
<td>Ray (1992)</td>
<td>[7]</td>
</tr>
<tr>
<td>Utilizing a modified configuration of SMBR for the OCM reaction</td>
<td>Tonkovich, et al. (1993)</td>
<td>[20,21]</td>
</tr>
<tr>
<td>A review of different chromatographic reactors</td>
<td>Sardin, et al. (1993)</td>
<td>[22]</td>
</tr>
<tr>
<td>A review of countercurrent and continuous chromatographic reactors</td>
<td>Carr, et al. (1993)</td>
<td>[23]</td>
</tr>
<tr>
<td>Acetic acid and β-phenyl alcohol esterification in an SMBR</td>
<td>Kawase, et al. (1996)</td>
<td>[10]</td>
</tr>
<tr>
<td>Modification of SMBR for OCM reactions</td>
<td>Kruglov, et al. (1996)</td>
<td>[26]</td>
</tr>
<tr>
<td>Experimental evaluation of esterification reaction in an SMBR</td>
<td>Mazzotti, et al. (1996)</td>
<td>[9]</td>
</tr>
</tbody>
</table>
in order to enhance separation efficiency of SMB operation.

On the other hand, for a catalytic reaction in gas phase at high pressure, it is possible to make use of pressure swing together with a SMBR process. At high pressure, while the reaction is progressing, and after some separation has occurred, the desorvent must be regenerated. For this reason, first the pressure must be decreased and then des sorption will start.

In Figure 2, a new configuration for Simulated Moving Bed Reactor together with Pressure Swing Adsorption (i.e., SMBR-PSA) is demonstrated. Two kinds of carrier gas, one in high (equal to operating) and the other in low (atmospheric) pressure, are employed in this pattern. According to the presented configuration, a complete cycle of the process contains six steps including: 1) Extract removal, 2) Elution by carrier gas, 3) Raffinate removal and simultaneous reaction and separation (or conventionally termed feed step), 4) Pressurization, 5) Purge and 6) Blowdown. All of these steps are included in one column, except the feed step. The number of columns in this step depends upon operational circumstances and must be optimized.

In the feed step, a mixture of reactants with a proper feed ratio at a high pressure enters into the column. The catalytic reaction goes forward and a mixture of products and reactants is subsequently formed. Since each component has different adsorption affinity (particularly at high pressures), the more strongly adsorbed species move slower, while the more weakly sorbed component breakthrough sooner, thus, eluting from the column as a raffinate stream. The elution by carrier gas step (i.e., feed column in previous step) contains a major part of more strongly adsorbed components and part of more weakly sorbed species. At this time, the weakly adsorbed components (e.g., unreacted species) are eluted by a high pressure carrier gas and added to feed which is entering into the feed column. It is very important that after this combination, a proper ratio of reactants is introduced into the feed column. According to the principles of SMB operation, after discharging less strongly adsorbed species into the feed column, just before the strongly sorbed component would leave the elution column, all inlet and outlet port advancements in direction of the fluid flow should take place. Therefore, switching time must be evaluated between breakthrough times of two key components from the elution column. The separating boundary is located between these components, in other words the most strongly adsorbed component in the raffinate and the most weakly adsorbed one in the extract stream.

After proper displacement of streams, a high pressure carrier gas causes exiting of the more strongly sorbed species from the extract removal column (i.e., elution column in the previous step). Next, the blowdown column (i.e., the end column of the raffinate removal section in the previous step) is discharged to

![Figure 2. SMBR-PSA configuration.](image-url)
the atmosphere in order to be prepared for regeneration at low pressure through the next step. The low pressure carrier gas enters into the purge column to remove the residue of the more strongly adsorbed components and prevent their build up on the adsorbent. Thus, the column is cleaned up and prepared for the next reaction and separation step. After this stage, a high pressure carrier gas is utilized to pressurize the column up to the operating amount needed in the pressurization step.

The presented SMBR-PSA configuration has some key parameters which affect the desired operation. These include switching time, selectivity of adsorbent, differences between breakthrough time of key components, number of columns in the reaction-separation step, flow rates of the streams, particularly feed and carrier gas of elution step and proper ratio in the feed make up through the feed column. Therefore, it is best to evaluate such systems experimentally.

**EXPERIMENTAL SECTION**

**Preliminary Experiments**

In order to evaluate the developed configuration of SMBR-PSA, one needs to first, select a proper catalyst and adsorbent. The catalytic hydrogenation of CO, that is termed Fischer-Tropsch Synthesis (FTS), is a gas phase reaction which goes forward at high pressure and is also compatible with SMBR-PSA idea. It is possible to produce a variety of hydrocarbon products, such as paraffins, olefins, aromatics and oxygenated components. The catalyst and operating conditions define the specific product. In this research, C₂ hydrocarbons (i.e., ethylene and ethane) have been chosen as desired products of the FTS. For this purpose, some catalysts with Fe, Cu and Mn as an active metal, and ZSM5, 5A molecular sieve and Y-zeolite as a support were made and tested in different operating conditions in a fixed bed reactor experimentally. According to the optimum operating conditions evaluated experimentally include, \( P = 18 \text{ bar}, T = 280^\circ \text{C}, \frac{\text{CO}}{\text{H}_2} = 0.773 \) and He (i.e., carrier gas) flow rate = 0.580 nml/s [27,28]. Reaction products over the selected catalyst at optimized conditions are CH₄, C₂ (i.e., C₂H₆ and C₂H₄) and CO₂.

Nevertheless, it is necessary to use a proper adsorbent for a good separation. Thus, some experiments were performed to select the best amongst available adsorbents. In Figure 3, breakthrough curves for four major components (i.e., CO, CO₂, CH₄ and C₂H₄) over two adsorbents, 5A molecular sieve and activated carbon (L’Air liquid), are illustrated. Based on the performed experiments for determining the isotherm and breakthrough curves, the 5A molecular sieve demonstrated a better capability to separate these components [28].

**Experimental Set up**

The configuration of SMBR-PSA pilot unit designed and constructed in the laboratory is shown schematically in Figure 4. The experimental apparatus is employed to monitor the progress of the FTS reaction and separate reactants and products simultaneously to enhance C₂ productivity and purity. The apparatus consists of eight columns co-packed with the adsorbent (i.e., 24.1 gr of 16/30 mesh 5A molecular sieve) and selected catalyst (i.e., 6.6 gr of 16/30 mesh). The length of each stainless steel column was 38 cm with a 12 mm inside diameter. The ends of the columns were fitted with a proper connection to 1/8 in swagelok unions and were packed with glass wool to hold solid particles in place. All connections between columns were made with 1/8 in. OD stainless steel tubing. All columns were located in an electrical heater that should be heated up to 450°C. The temperature is measured by a thermocouple in the thermowell that is embedded in each column and controlled by a TLC.

Several solenoid valves are used to accomplish switching of entering streams, including make-up feed, high and low pressure carrier gas and exiting streams. These include extract and raffinate products, vent and stream to the next column. Seven solenoid valves (Rapa Germany, size 1/8 in.) were used for each column to direct the gases to enter and exit the appropriate column. The valve diagram, which is identical for all columns, is presented in Figure 5. The position of all the 56 solenoid valves is controlled by a personal computer IBM/80-486 for data acquisition and process sequencing control, equipped with a data translation and a series of solid state relays.

The precise flow rate of input gases are indicated and controlled by mass flow meter / controller (Brooks
A Shimadzu GC-6PT gas chromatograph with a Thermal Conductivity Detector (TCD) is used to measure effluent gas concentrations. This GC is connected to the computer for data processing.

**Experimental Procedure and Results**

In order to verify the aforementioned SMBR-PSA idea, it was necessary to run appropriate tests. Also, it was very important to design experiments in order to find the optimum parameters for successful operation. Certainly, breakthrough times for different components are the most important variables in these systems. They should be used to determine the switching time, which is a key parameter in this process.

The dynamic response of the reactor for the catalyst and then the mixture of catalyst and adsorbent being co-packed in a bed should be evaluated. Finally, after estimating optimum parameters, a complete cycle of SMBR-PSA will be run to investigate the system capability for simultaneous reaction and separation. Since SMBR-PSA operation is affected by transient behavior, due to switching of streams alternatively, dynamic response of catalyst should be evaluated.

Test of the dynamic response of the catalyst is performed in an individual reactor. The selected catalyst is loaded, then optimum operating conditions which were determined at prior steady state concentration tests, are set. For each experiment, the catalyst and adsorbent have been regenerated by a mixture of 90% He and 10% H₂, with 11.7 n/br total flow, for 17 hours at 450°C. The stream of reactants (i.e., CO= 0.194 and H₂ = 0.251 nml/s) is allowed to enter into the reactor (i.e., t = 0) and then 11 samples are taken and reserved from the outlet of this reactor at pre-determined intervals. Ultimately, the transient response of the reactor is obtained by GC analysis of these samples.

Figure 6 shows the composition variation of components from the transition up to steady state period. These results indicate that CO content in the effluent stream has an increasing trend. At initial operation period, when the reactor is still clean, the catalyst has a higher activity. Therefore, CO conversion shows a decreasing trend and ultimately reaches down the steady state plateau as time goes by. Hydrocarbons produced here are mainly based upon the four reactions on the iron catalyst as follows:

\[
\begin{align*}
\text{CO} + 3\text{H}_2 & \rightarrow \text{CH}_4 + \text{H}_2\text{O} \\
\text{CO} + 5/2\text{H}_2 & \rightarrow 1/2\text{C}_2\text{H}_6 + \text{H}_2\text{O} \\
\text{CO} + 2\text{H}_2 & \rightarrow 1/2\text{C}_2\text{H}_4 + \text{H}_2\text{O} \\
\text{CO} + \text{H}_2\text{O} & \Leftrightarrow \text{CO}_2 + \text{H}_2
\end{align*}
\]

It is observed that CO₂ is produced from reaction D.
Simulated moving bed section

Low pressure
carrier gas

TO GC

Gas no 1

Gas no 2

High pressure
carrier gas

Legend

- Pressure reducing
  valve
- Back pressure
  relief valve
- Needle valve
- Ball valve
- Check valve
- Dust filter
- 3 way ball
  valve
- Solenoid valve

Vent

Heater power
Supply

Reactor

Condensate

CO$_2$H$_2$ = 0.773, GHSV = 528 (1/hr), $T = 280^\circ$C, $P = 18$ bar

Figure 6. Dynamic analysis for catalyst in the reactor.

(Also known as the Water Gas Shift or WGS reaction)
and effected by H$_2$O production in other reactions.
Thus, increasing of CO$_2$ and decreasing of CH$_4$, C$_2$H$_6$
and C$_2$H$_4$ through time may be reasoned out.

In order to determine the share of each reaction
in the overall production scheme presented by the
above mechanism, one may use the results of the
dynamic testing in addition to the overall material
balance. The results of these calculations, summarized
in Table 2, indicate that increasing the CO$_2$ production
(i.e., D reaction) causes a decrease in hydrocarbons
production. The backward reaction in the WGS helps
to produce CO which inturn causes an increase in CH$_4$
production up to the steady state concentration. It is
seen from Figure 6 that the dead time of this system is
about 100 seconds and after 140 seconds concentration
of all species will approach their steady state amounts.

In the next set of experiments, the transient
response for a column of SMBR-PSA system, which
is loaded with a mixture of catalyst and adsorbent, is
determined. All operating conditions and experimental
procedures are applied just as before. Figure 7 shows
the obtained results of GC analysis for 11 samples
taken from the effluent stream of the aforementioned
column at pre-determined times. Although these
results display similar trends as previous ones, dead
and breakthrough times for species in the latter case
are shorter. This is due to the fact that this column
possesses a smaller volume than the reactor. The
dead time of 30 seconds and necessary time to arrive
Table 2. The share of each main FTS reactions in the overall production scheme.

<table>
<thead>
<tr>
<th>Loop No.</th>
<th>Time (s)</th>
<th>CO%</th>
<th>CH₄%</th>
<th>CO₂%</th>
<th>C₂%</th>
<th>X%</th>
<th>A%</th>
<th>B + C%</th>
<th>D%</th>
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<td>---</td>
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<tr>
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<td>---</td>
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<td>64.54</td>
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</table>

![Graph](image1.png)

**Figure 7.** Dynamic response for a mixture of catalyst and adsorbent in a column.

at the steady state concentration of 80 seconds after introducing the feed into the column is seen in the outlet. CO, CO₂ and C₂ appear in the effluent stream after 40, 50 and 60 seconds, respectively. This is related to the reaction kinetics and the adsorbent-chemical species interactions.

Because of these results and based on the main purpose of this research, an appropriate separating boundary should be considered. According to the obtained results in this work, the best position for the separating boundary, in order to distinguish unreacted feed and products, is to locate it between the column for CH₄ and CO species are close to each other, yet different from CO₂ and C₂ products. It should be reiterated that the aim of this study is to produce and separate C₂ components. Thus, the extract stream will be concentrated with C₂ and CO₂, while the raffinate stream is purified with CH₄ and CO. The location of the separating boundary is, ultimately, specified by the switching time. The proper switching time allows only for the passage and entrance of raffinate components into the next column. From these results, it is predicted that switching time should be in the range of 30 to 50 seconds in this system.

![Graph](image2.png)

**Figure 8.** Dynamic analysis of which three consecutive columns co-packed catalyst and adsorbent.

The difference in breakthrough time for components in one column is not sufficient to have a good separation and the desired purification. In order to omit this problem, one may increase the number of reaction and separation columns in this system.

Through the next run of experiments, three columns co-packed with catalyst and adsorbent are employed. All of the process circumstances are as before. The dynamic analysis for three consecutive columns is illustrated in Figure 8. From these results, dead time is about 100 seconds. Methane, as a main product, with the shortest residence time is eluted first followed by CO, CO₂ and C₂ at 130, 140 and 150 seconds, respectively. These results indicate that by increasing the number of columns, one may achieve a better separation.

On the other hand, increasing the number of columns causes a decrease in the unreacted CO and an increase in the undesired CO₂ product of the effluent stream. This is related to the WGS reaction progress when the H₂O is produced and reacted with CO in the column. Also, the hydrocarbon reactions are prevented from occurring due to lack of hydrogen content in these columns. Therefore, further increase in the
number of columns decreases the selectivity of the desired products. Thus, it is a foregone conclusion that there would be a trade-off between a good selectivity and separation when employing optimum number of columns. In order to compare results of these cases, selectivity and yield of products at the steady state situation are shown in Table 3. Therefore, based on these findings, a system of three mixed columns in series is proposed in order to obtain a better yield for C₂ products.

In order to evaluate SMBR-PSA scheme, a complete cycle of the process based on obtained results and optimum parameters is tested. The reaction and separation steps include three columns; therefore, accounting for the five steps previously described, the total number of columns needed is eight. All eight columns are loaded with 6.6 gr of catalyst and 24.1 gr of adsorbent, similar to previous tests. The same operating conditions including $T = 280^\circ$C, $P = 18$ bar and elution carrier gas flow rate equal to 0.580 nml/s are utilized.

After regeneration of the catalyst and adsorbent and initial preparation, the feed stream containing CO and H₂ with flow rates of 0.194 and 0.251 nml/s, respectively, is introduced into the feed column. The stream switching and sequencing system is set by entering the position of solenoid valves and switching times into an interfaced PC with the system for this purpose. Since a part of unreacted CO will exit from the elution step and add to the feed, the amount of CO should be decreased in the make-up feed. After many experiments, 0.175 nml/s is determined to be a suitable flow rate of CO. Thus, the process starts up with 0.194 nml/s for CO flow rate and decreases rapidly to 0.175 nml/s after the first switching.

In order to analyze product streams, five samples are taken from each of the extract and raffinate streams, at pre-determined times for second through sixth cycles. Experiments are fulfilled for 30, 40 and 50 seconds switching times. Figures 9 and 10 show the analysis of the extract and raffinate streams for the switching time of 30 seconds. It is seen that a part of the raffinate stream (containing CH₄ and CO) cannot come out of the elution column, hence contaminating the extract stream.

In Table 4, the amount of different components in the extract stream versus the switching time is
Table 4. Variation of mole percent of different components versus $t_s$ in the extract stream.

<table>
<thead>
<tr>
<th>$t_s$</th>
<th>CO</th>
<th>CH$_4$</th>
<th>CO$_2$</th>
<th>C$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>5.08</td>
<td>8.35</td>
<td>46.20</td>
<td>40.37</td>
</tr>
<tr>
<td>40</td>
<td>2.07</td>
<td>3.52</td>
<td>47.51</td>
<td>46.90</td>
</tr>
<tr>
<td>50</td>
<td>0</td>
<td>2.77</td>
<td>54.26</td>
<td>42.97</td>
</tr>
</tbody>
</table>

displayed. As is observed, the best purity of C$_2$ components is obtained at $t_s = 40$ s. Also, in Table 5, the recovery of C$_2$ components in the extract stream versus the switching time is illustrated. According to these results, it is a foregone conclusion that with an increase in switching time, even though the recovery of desired products is decreased, the best separation results is obtained at $t_s = 40$ s.

It is a good idea to compare SMBR-PSA results with those of a Fixed Bed reactor (FB). In Table 6 the ratio of the outlet components of the SMBR-PSA (i.e., extract and raffinate streams) to those of an FB at similar conditions are presented. It is observed that despite the reduction of CO introduced into the feed column from 0.194 to 0.175 nmol/s, the amount of unreacted CO in the outlet is lower in SMBR-PSA compared with that of an FB. It may also be seen that due to an increased CO conversion, all products have an increase in yield. Furthermore, the selectivity of CO$_2$ has a more pronounced increase than other species. Ultimately, according to this table, the best results to produce desired products is expected to appear at $t_s = 40$ s, where an increase of 10 percent in the amount of these species is reached.

CONCLUSIONS

In this study, the feasibility of SMB application to the simultaneous gas phase reaction and separation has been determined experimentally. For this purpose, a new configuration including a combination of SMBR and PSA has been employed and verified through experiments. Moreover, some guidelines for optimization of the process have been discussed.

Although this technique needs more complicated controllers (for stream switching) and uses a lot of gas (as a carrier or purge), it has many advantages over
Table 5. The recovery of components in the extract stream versus the switching time.

<table>
<thead>
<tr>
<th>$t_s$ (s)</th>
<th>(CO)<em>{ext}/(CO)</em>{SMB}</th>
<th>(CH_4)<em>{ext}/(CH_4)</em>{SMB}</th>
<th>(CO_2)<em>{ext}/(CO_2)</em>{SMB}</th>
<th>(C_2)<em>{ext}/(C_2)</em>{SMB}</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>0.223</td>
<td>0.036</td>
<td>0.691</td>
<td>1.000</td>
</tr>
<tr>
<td>40</td>
<td>0.082</td>
<td>0.012</td>
<td>0.580</td>
<td>0.872</td>
</tr>
<tr>
<td>50</td>
<td>0</td>
<td>0.007</td>
<td>0.494</td>
<td>0.618</td>
</tr>
</tbody>
</table>

Table 6. Product ratio of SMBR-PSA to fixed bed reactor.

<table>
<thead>
<tr>
<th>$t_s$ (s)</th>
<th>(CO)<em>{SMB}/(CO)</em>{FB}</th>
<th>(CH_4)<em>{SMB}/(CH_4)</em>{FB}</th>
<th>(CO_2)<em>{SMB}/(CO_2)</em>{FB}</th>
<th>(C_2)<em>{SMB}/(C_2)</em>{FB}</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>0.285</td>
<td>1.18</td>
<td>1.45</td>
<td>1.02</td>
</tr>
<tr>
<td>40</td>
<td>0.256</td>
<td>1.18</td>
<td>1.43</td>
<td>1.10</td>
</tr>
<tr>
<td>50</td>
<td>0.264</td>
<td>1.18</td>
<td>1.44</td>
<td>1.07</td>
</tr>
</tbody>
</table>

fixed beds. Ultimately, from the work described above, the following conclusions may be drawn:

1. The use of unreacted materials without utilizing of the recycle stream causes an increase in reaction conversion in a smaller column of SMBR-PSA compared with that of a fixed bed. It has been realized through SMBR-PSA technology that in spite of decreasing COin the make-up feed, the conversion rises up, due to the use of reactants in columns ahead;

2. All product yields increase with increasing the reaction conversion in the SMBR-PSA process. However, due to reaction kinetics and dynamics of the system, different products show different elevation in their yields. It is obvious that all products have higher yields in SMBR-PSA setting, however, the CO_2 has the most noticeable extent. This should be related to the reversibility of the WGS reaction, which produces CO_2. Therefore, it is demonstrated that due to simultaneous reaction and separation, reversible reactions progress further than their irreversible counterparts;

3. The split of products into two streams (i.e., raffinate and extract) is yet another important advantage of SMBR-PSA process. The combination of separation and reaction sections has an effective role in process cost reduction. Thus, it is realized that with correct selection of effective parameters, one may achieve a highly successful process.

REFERENCES


