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Fractional Factorial Design Study of a Pressure Swing Adsorption-Solvent Vapor Recovery Process

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Abstract. A two-level fractional factorial study was performed by computer simulation on the periodic state process performance of a pressure swing adsorption-solvent vapor recovery process (PSA-SVR). The goal was to investigate factor (parameter) interaction effects on the process performance, i.e., interaction effects that cannot be ascertained from the conventional "one-at-a-time" approach. Effects of seven factors, i.e., the purge to feed ratio, pressure level, pressure ratio, heat transfer coefficient, feed concentration, feed volumetric flow rate and bed length to diameter ratio, on the process performance were investigated. The results were judged in terms of the light product purity, heavy product enrichment (and relative enrichment) and recovery, and bed capacity factor. Only the purge to feed ratio, pressure ratio, and feed concentration had significant effects on the benzene vapor enrichment (and relative enrichment); and no two-factor and higher interactions were observed. The light product purity was affected by all seven factors; and the relative importance of the effect of each factor depended on the levels of the other factors, i.e., significant two-factor interaction effects existed. Two-factor interaction effects also existed on the benzene vapor recovery, although the effects of all seven factors and their interactions were relatively small. The bed capacity factor was affected mainly by the purge to feed ratio, the heat transfer coefficient and the feed concentration; two factor and higher order interaction effects were insignificant. Overall, this study demonstrated the utility of fractional factorial design for revealing factor interactions and their effects on the performance of a PSA-SVR process.

Keywords: pressure swing adsorption, environmental, activated carbon, simulation, factorial design

Introduction

The pressure swing adsorption (PSA)-solvent vapor recovery (SVR) process has been overlooked by industry, until only recently. However, the recent commercialization of this process has changed this lack of interest (Holman and Hill, 1992; Hall and Larrinaga, 1993). A variety of commercial applications of PSA-SVR have proved its efficiency and economy compared to conventional solvent vapor recovery processes. Its important environmental applications include the recovery and concentration of organic vapors produced from wastewater collection and treatment operations, process vents, gasoline storage vessel vents, etc. However, what sets PSA-SVR apart from conventional PSA processes is that the performance is based on the light product purity (usually air), and the enrichment and recovery of the heavy component (i.e., the solvent vapor). In contrast, conventional PSA process performance is judged by the light product purity and recovery, while the heavy component is simply an undesirable waste gas; and over the past two decades, the industrial and academic focus on the development of most PSA processes has been only on the purification and recovery of the light component. Thus, the understanding of PSA for heavy product enrichment and recovery is lacking.

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The recent works by Ritter and Yang (1991a,b) appear to have been the first PSA studies to address the simultaneous light component purification, and heavy component recovery and enrichment both experimentally and theoretically. Following their works, PSA researchers began investigating heavy component enrichment and recovery from a variety of feed gases (Kikkinides et al., 1991; Kikkinides and Yang, 1991, 1993a,b; Diagne et al., 1994, 1995; Chue et al., 1995; Liu and Ritter, 1996). These studies collectively showed that the PSA-SVR process performance is affected by many factors (parameters), including the process and operating conditions, and the bed dimensions. The effects of some important factors on the process performance have been investigated by Ritter and Yang (1991a), Chue et al. (1995) and Diagne et al. (1995), with the most comprehensive study done by Liu and Ritter (1996). They investigated the effects of nine parameters on the performance of a PSA process designed for benzene vapor recovery. However, all of these studies have taken the familiar "one-at-a-time" approach, in which all factors are held constant while one factor is varied, and this process is repeated for each remaining factor. Although this approach may appear very logical, as the comparisons are made under relatively homogenous conditions, it is incapable of assessing the relative importance of each factor and measuring the extent of interactions between various factors. In many situations factors interact with each other so that the performance of the process (responses) depends on the particular factor level combinations employed.

In view of the various factors contributing to the PSA-SVR process performance, it is difficult to assess the relative importance of each factor without a systematic approach to the problem. Factorial design is proving to be a very powerful technique when dealing with this kind of problem. For example, Bohn and Manz (1985) used a 2^4 factorial design to examine the interaction effects of various reactor parameters on the properties of SiNH films; Kannan et al. (1988) used a one-eighth fractional design to optimize a porous-carbon fuel-cell electrode; and Gaertner and Dhurjati used a one-sixteen fractional factorial design to identify important variables and variable interactions affecting the hybridoma reaction system (1993a) and a one-half fractional factorial to identify the important variables and interactions affecting the kinetics of nutrient uptake and waste production (1993b).

A factorial design was used here to carry out, by computer simulation, a systematic and extensive study on the effects of seven of the most important parameters (factors) on the PSA-SVR process performance. The seven factors (parameters) were: the purge to feed ratio (PF), pressure level (PL), pressure ratio (PR), heat transfer coefficient (H), feed molar fraction (YF), feed volumetric flow rate (VF), and bed length to diameter ratio (LD). The process performance was based on the solvent vapor recovery (R), enrichment (E), relative enrichment (E_R), light product purity (y_p), and bed capacity factor (BCF). The overall objective was to obtain a comprehensive understanding of the relative importance of the effects of each factor on the process performance, and the effects of their interactions, if any, which could not be gleaned from the aforementioned "one-at-a-time" studies.

Process Description and Process Performance Indicators

Process Description

A four-step, two-bed, PSA-SVR process was simulated in this study using commercially relevant PSA-SVR process conditions for the recovery of benzene vapor from nitrogen (inert carrier gas) using activated charcoal. The four steps consisted of (I) cocurrent feed pressurization from P_L to P_H, (II) cocurrent high pressure adsorption with feed, (III) countercurrent blowdown from P_H to P_L (evacuation), and (IV) low pressure desorption with countercurrent light product purge. Note that since high affinities exist between the solvent vapor and the adsorbent, vacuum desorption was necessary in Step IV. The solvent vapor was enriched and recovered in Steps III and IV, whereas the light component was purified during Step II. In Step IV the purge gas used in one bed came directly from the other bed as the light product of Step II; thus, the inlet purge gas of one bed had the same composition and temperature as the Step II light product of the other bed at all times. The amount of the light product that was used for purge was determined by the PF, which was defined as the ratio of the actual gas volume used for purge to the actual volume of the feed gas. In special cases, as in the present study, where the adsorption step time is equal to the purge step time, PF is equal to the ratio of the purge gas velocity at P_L to the feed gas velocity at P_H.

The seven factors were changed as follows. The PF was increased by increasing the purge flow rate during

Step IV. The PL was changed by changing both the high and low pressures, and it was represented by P_L. The pressure ratio was changed by decreasing P_L with P_H fixed. The H was simply increased to a different value, as was the VF. The LD was changed while keeping the bed volume constant.

Process Performance Indicators

The PSA-SVR process performance at the periodic state was judged by five process performance indicators: R, E and E_R, y_p, and the BCF. R was defined as the ratio of the number of moles of the solvent vapor leaving the bed during Steps III and IV to the number of moles of the solvent vapor entering the bed during Steps I and II. E was defined as the average mole fraction of the solvent vapor leaving the bed during Steps III and IV divided by the mole fraction of the feed solvent vapor. E_R was defined by Liu and Ritter (1996) as the ratio of the actual E to the maximum possible enrichment obtained under the most ideal conditions (E_I). The most ideal conditions exist when heat and mass transfer, and velocity effects are ignored, the gas and adsorbed phases are frozen during Steps I and III, the bed is long enough to contain the concentration wave, and the purge to feed ratio is unity (LeVan, 1995). Liu and Ritter (1996) showed that under these conditions, E_I is simply equal to P_H/P_L, and that E_I provides a fixed reference point from which to judge E. y_p was defined as the average mole fraction of the solvent vapor exiting the light product end of the bed during Step II. BCF was defined as (Liu and Ritter, 1996)

$$\mathrm{BCF} = \int_0^L q \, dz / q_f^* L \tag{1}$$

BCF represents the capacity of the bed that is used at the periodic state (measured at the end of Step II) compared to the maximum capacity of the bed at the feed conditions. Thus, at a fixed process throughput and when there is no solvent vapor breaking through the bed during Step II, a higher BCF indicates a poorer performance.

Mathematical Model

The mathematical model used in this study was the same as that used in a previous study (Liu and Ritter, 1996) and is summarized briefly below. The assumptions were inert carrier gas and adsorbent; single component feed; negligible column pressure drop; ideal gas behavior; no radial gradients, and no axial dispersion and heat conduction; thermal equilibrium between gas phase and adsorbent; and temperature-independent gas and adsorbent properties. The mass and heat transfer were accounted for by using, respectively, the linear driving force (LDF) approximation, and an overall heat transfer coefficient.

The total and component mass balances were given by

$$\frac{\partial y}{\partial t} + u\frac{\partial y}{\partial z} + (1-y)\frac{(1-\varepsilon)}{\varepsilon}\frac{RT}{P}\rho_s\frac{\partial q}{\partial t} = 0 \tag{2}$$

$$\frac{\partial u}{\partial z} - \frac{1}{T}\frac{\partial T}{\partial t} + \frac{1}{P}\frac{\partial P}{\partial t} - \frac{u}{T}\frac{\partial T}{\partial z} + \frac{(1-\varepsilon)}{\varepsilon}\frac{RT}{P}\rho_s\frac{\partial q}{\partial t} = 0 \tag{3}$$

where $\partial q/\partial t$ was based on the LDF approximation as

$$\frac{\partial q}{\partial t} = k(q^* - q) \tag{4}$$

The energy balance was given by

$$\left(\rho_g C_{p_g} + \frac{1-\varepsilon}{\varepsilon}\rho_s C_{p_s}\right)\frac{\partial T}{\partial t} + \rho_g C_{p_g}\left(u\frac{\partial T}{\partial z} + T\frac{\partial u}{\partial z}\right) + \Delta H\frac{1-\varepsilon}{\varepsilon}\rho_s\frac{\partial q}{\partial t} + \frac{2H}{\varepsilon r_b}(T - T_0) = 0 \tag{5}$$

Equations (6) and (7) denote the temperature dependent adsorption equilibria for the nitrogen-benzene vapor-activated charcoal system.

$$q^* = \frac{q_s b P y}{1 + bPy} \tag{6}$$

$$b = \frac{b_0}{R\sqrt{T}}\exp\left(-\frac{\Delta H}{RT}\right) \tag{7}$$

The initial and boundary conditions are listed below; they were applied to every cycle:

$$\begin{array}{llll}
\text{Step I:} & \text{at } t = 0: & y = y_{\mathrm{IV}},\ T = T_{\mathrm{IV}}, & \\
 & & q = q_{\mathrm{IV}} & \text{for all } z \\
 & \text{at } z = 0: & y = y_f,\ T = T_f & \text{for all } t \\
 & \text{at } z = L: & u = 0 & \text{for all } t \\
\text{Step II:} & \text{at } t = 0: & y = y_{\mathrm{I}},\ T = T_{\mathrm{I}},\ q = q_I & \text{for all } z \\
 & \text{at } z = 0: & y = y_f,\ T = T_f,\ u = u_f & \text{for all } t \\
\text{Step III:} & \text{at } t = 0: & y = y_{\mathrm{II}},\ T = T_{\mathrm{II}},\ q = q_{\mathrm{II}} & \text{for all } z \\
 & \text{at } z = L: & \partial y/\partial z = 0,\ u = 0 & \text{for all } t \\
\text{Step IV:} & \text{at } t = 0: & y = y_{\mathrm{III}},\ T = T_{\mathrm{III}}, & \\
 & & q = q_{\mathrm{III}} & \text{for all } z \\
 & \text{at } z = L: & y(t) = y_{\mathrm{II}}(t), & \\
 & & T(t) = T_{\mathrm{II}}(t),\ u = u_P & \text{for all } t
\end{array}$$

Table 1. Bed characteristics, fixed process conditions, and physical properties.

Bed diameter	0.027 m
Bed length	0.29 m
Bed void fraction	0.43
Solid density	480 kg/m^3
Heat capacity of adsorbent	1.05 kJ/(kg K)
Feed temperature	293 K
Ambient temperature	293 K
Total cycle time	20 min
Cycle step time I and III:	2 min
II and IV:	8 min
Gas phase density	1.308 kg/m^3
Gas phase heat capacity	1.006 kJ/(kg K)
Heat of adsorption	−43.5 kJ/mol
Mass transfer coefficient	0.086 1/s
q_s	4.4 mol/kg
b_0	3.88 e^{-8} m^3/(mole K$^{0.5}$)

Table 2. Factors investigated and their levels*.

Levels	PF (—)	PL (kPa)	PR (—)	H kJ/(m^2 s K)	YF (%)	VF × 10^6 (m^3 STP/s)	LD (—)
Low (−)	1.5	5.5715	20.0	0.004184	2.5	400.0	5.0
High (+)	2.0	7.5975	30.0	0.02092	5.0	500.0	10.74

*(−) represents the low level and (+) represents the high level.

The pressure history was required as input to the PSA model. The pressure history was represented by a linear function of time during Steps I and III; and it was held constant at P_H and P_L during Steps II and IV, respectively. The bed characteristics, together with the fixed operating conditions and physical properties, are given in Table 1. Details of the solution method are given elsewhere (Liu and Ritter, 1996); finite differences were employed along with an appropriate matrix solver.

Fractional Factorial Design of Simulations

A full factorial design is an experimental (or simulation) arrangement in which a small integral number of levels, l, is chosen for each of k factors, and all l^k combinations of these levels are run. Clearly, the major disadvantage of the full factorial method is that the number of trial runs required increases geometrically with k. For example, the present study utilized two levels ($l = 2$) for seven factors ($k = 7$); the full 2^7 factorial design would have required 128 trial runs. These runs would be comprised of one average effect, seven main effects, twenty-one two-factor interaction effects, thirty-five three-factor interaction effects, thirty-five four-factor interaction effects, twenty-one five-factor interaction effects, seven six-factor interaction effects, and one seven-factor interaction effect. Fortunately, however, it is possible to reduce the number of runs quite substantially by confounding the higher order interactions with the individual factors. This kind of factorial design is called fractional factorial design and was first proposed by Finney (1945). The detailed theoretical basis of this design is beyond the scope of this study; information can be found in the works by Finney (1945) and Dey (1985).

In general, main factors tend to be more important than two-factor interactions, which tend to be more important than three-factor interactions, etc. Physically, higher order interactions are expected to be less significant. Therefore, by properly designing the fractional factorial simulation and letting the main factors be confounded with only higher order interactions, the confounded effects can be interpreted approximately as the main effects only.

The effects of the seven factors mentioned previously on the PSA-SVR process performance were investigated in the present study ($k = 7$). Two levels ($l = 2$) were used for each of the seven factors. The factors and their levels are summarized in Table 2. A one-eighth fraction (l^{-3}) of the 2^7 full factorial design was used, which is called a 2^{7-3} fractional factorial design (Box et al., 1978; Duckworth, 1986). Furthermore, a 2^{7-3} fractional factorial design of resolution IV was used, which means that no main effects (or effect of the individual factor) are confounded with each other or with two-factor interaction (second order interaction) effects; but the main effects may be confounded with the third and higher order interaction effects, and any interaction effects may be confounded. Experience has shown that real interaction effects are not likely to occur unless at least one of the factors involved in the interaction has a main effect; and only rarely are significant higher than two-factor interactions observed (Lochner and Matar, 1990).

Results and Discussion

The resolution IV, 2^{7-3} fractional factorial design matrix is given in Table 3, along with the PSA-SVR process performance (responses) for each of the 16

Table 3. Design matrix and process performance responses.

	Factor levels							Process performance responses				
Run No.	PF	PL	PR	H	YF	VF	LD	E (—)	E_R (—)	y_p (ppm)	R (%)	BCF (%)
1	−	−	−	−	−	−	−	8.017	0.401	0.0	100.0	70.935
2	−	−	−	+	−	+	+	8.192	0.410	0.0	100.0	54.903
3	−	−	+	−	+	−	+	6.786	0.226	1500.4	97.359	99.831
4	−	−	+	+	+	+	−	7.116	0.237	1187.5	97.897	99.836
5	−	+	−	−	+	+	−	5.056	0.248	14466.0	74.146	99.992
6	−	+	−	+	+	−	+	6.303	0.315	34.96	99.941	99.345
7	−	+	+	−	−	+	+	10.281	0.343	0.12	99.999	91.916
8	−	+	+	+	−	−	−	10.197	0.340	0.00	100.0	56.956
9	+	−	−	−	+	+	+	4.859	0.243	1793.1	96.943	99.792
10	+	−	−	+	+	−	−	5.452	0.273	0.00	100.0	83.987
11	+	−	+	−	−	+	−	8.404	0.280	0.00	100.0	72.119
12	+	−	+	+	−	−	+	8.540	0.285	0.00	100.0	35.543
13	+	+	−	−	−	−	+	6.403	0.320	0.00	100.0	48.777
14	+	+	−	+	−	+	−	6.541	0.327	0.00	100.0	44.207
15	+	+	+	−	+	−	−	5.814	0.194	1.92	99.997	99.394
16	+	+	+	+	+	+	+	6.260	0.209	290.2	99.503	99.737
Average response (grand mean)								7.139	0.291	1204.6	97.863	78.579

runs. In addition to these performance indicators for each trial run, the average responses (grand means) are also listed in the last row of Table 3. It must be emphasized that the effects of the factors can not be judged in terms of the responses of any individual trial run, i.e., the individual responses in Table 3 have little meaning in distinguishing the significant effects. Table 4 gives the average responses at the low and high levels of the factors and interactions, and the effect of each factor and interaction on the process performance. Table 5 gives the alias structure of this design. The alias of a factor or interaction consists of the additional factors or interactions that are confounded with the factor or interaction in question. For example, the effects of the PF-PL interaction given in Table 4 are actually the confounded effects of PF-PL and all of its alias given in Table 5, i.e., three two-factor interactions, four four-factor interactions, and one six-factor interaction. The "effect" of a factor or an interaction represents the average difference between a specific process performance indicator at the high and low levels of the factor or interaction. The sign with each effect indicates whether the factor or interaction has a "beneficial" or "adverse" effect on the process performance indicator.

To identify the confounded factors or interactions which have "significant" effects on the process performance, the normal plot technique was used (Box et al., 1978; Lochner and Matar, 1990). If there is no "real" factor or interaction effect, the estimated effects should have a distribution similar to that of a random sample from a normal population. When plotted on normal probability paper, these estimated effects should be in approximately a straight line. Effects which are real, on the other hand, should have estimates which appear too large or too small to be part of a normal random sample. On a normal plot, these estimates would be outside of the straight line pattern displayed by the bulk of the other points. This graphical approach of identifying "significant" estimates is useful because it provides some protection against identifying an effect as being real simply because it is larger, but not significantly larger, in magnitude than other estimated effects. Although the analysis of variance technique can also be used for this purpose and is more quantitative than the normal plot technique, it is not necessarily a better technique due to some of its weaknesses, as pointed out by Lochner and Matar (1990).

Table 4. Average performance indicators at high and low levels and magnitudes of effects*.

	Factors							Interactions								
	PF	PL	PR	H	YF	VF	LD	PF-PL	PF-PR	PF-H	PF-YF	PF-VF	PF-LD	PL-LD	PF-PL-LD
Low level E	7.743	7.171	6.353	6.952	8.322	7.189	7.075	7.387	7.204	7.161	6.894	7.107	7.222	6.998	7.184
High level E	6.534	7.107	7.925	7.325	5.956	7.089	7.203	6.891	7.073	7.117	7.384	7.171	7.056	7.279	6.998
Effect on E	−1.209	−0.064	1.572	0.373	−2.366	−0.1	0.128	−0.495	−0.131	−0.044	0.490	0.064	−0.166	0.281	−0.09
Low level E_R	0.315	0.294	0.317	0.282	0.338	0.294	0.288	0.291	0.289	0.292	0.280	0.289	0.296	0.284	0.293
High level E_R	0.266	0.287	0.264	0.300	0.243	0.287	0.294	0.291	0.293	0.289	0.302	0.293	0.285	0.297	0.288
Effect on E_R	−0.049	−0.007	−0.053	0.018	−0.095	−0.007	0.006	0.000	0.004	−0.003	0.022	0.004	−0.011	0.013	−0.005
Low level y_p (ppm)	2148	560	2036	2220	0.015	192	1957	2036	560	377	2148	1957	192	2220	377
High level y_p (ppm)	260	1849	372	189	2409	2217	452	372	1849	2032	260	452	2217	189	2032
Effect on y_p (ppm)	1888	1289	−1664	−2031	2409	2025	−1505	−1664	1289	1655	−1888	−1505	2025	−2031	1655
Low level R (%)	96.171	99.025	96.382	96.058	100.0	99.662	96.508	96.382	99.025	99.347	96.170	96.508	99.662	96.059	99.347
High level R (%)	99.556	96.701	99.344	99.668	95.726	96.064	99.218	99.345	96.701	96.379	99.555	99.218	96.064	99.668	96.379
Effect on R (%)	3.385	−2.324	2.963	3.610	−4.274	−3.598	2.710	2.963	−2.323	−2.969	3.385	2.710	−3.598	3.609	−2.968
Low level BCF (%)	84.214	77.118	75.242	85.345	59.419	74.346	78.428	79.956	78.163	78.89	74.956	76.793	80.713	73.827	80.121
High level BCF (%)	72.945	80.041	81.917	71.814	97.739	82.813	78.73	77.202	78.996	78.269	82.202	80.365	76.446	83.332	77.038
Effect on BCF (%)	−11.27	2.923	6.675	−13.53	38.32	8.467	0.302	−2.754	0.833	−0.622	7.246	3.572	−4.267	9.504	−3.083

*Refer to Table 5 for confounded interactions associated with each of the factors or interactions.

Table 5. Alias structure of the resolution IV, 2^{7-3} fractional factorial simulation design.

Factors or interactions (from Table 4)	Confounded interactions (Alias)
PF	PL-PR-YF, PL-*H*-VF, PR-*H*-LD,YF-VF-LD, PF-PL-PR-VF-LD, PF-PL-*H*-YF-LD, PF-PR-*H*-YF-VF
PL	PF-PR-YF, PF-*H*-VF, PR-VF-LD, *H*-YF-LD, PF-PL-PR-*H*-LD, PF-PL-YF-VF-LD, PL-PR-*H*-YF-VF
PR	PF-PL-YF, PF-*H*-LD, PL-VF-LD, *H*-YF-VF, PF-PL-PR-*H*-VF, PF-PR-YF-VF-LD, PL-PR-*H*-YF-LD
H	PF-PL-VF, PF-PR-LD, PL-YF-LD, PR-YF-VF, PF-PL-PR-*H*-YF, PF-*H*-YF-VF-LD, PL-PR-*H*-VF-LD
YF	PF-PL-PR, PF-VF-LD, PL-*H*-LD, PR-*H*-VF, PF-PL-*H*-YF-VF, PF-PR-*H*-YF-LD, PL-PR-YF-VF-LD
VF	PF-PL-*H*, PF-YF-LD, PL-PR-LD, PR-*H*-YF, PF-PL-PR-YF-VF, PF-PR-*H*-VF-LD, PL-*H*-YF-VF-LD
LD	PF-PR-*H*, PF-YF-VF, PL-PR-VF, PL-*H*-YF, PF-PL-PR-YF-LD, PF-PL-*H*-VF-LD, PR-*H*-YF-VF-LD
PF-PL	PR-YF, *H*-VF, PF-PR-VF-LD, PF-*H*-YF-LD, PL-PR-*H*-LD, PL-YF-VF-LD, PF-PL-PR-*H*-YF-VF
PF-PR	PL-YF, *H*-LD, PF-PL-VF-LD, PF-*H*-YF-VF, PL-PR-*H*-VF, PR-YF-VF-LD, PF-PL-PR-*H*-YF-LD
PH-H	PL-VF, PR-LD, PF-PL-YF-LD, PF-PR-YF-VF, PL-PR-*H*-YF, *H*-YF-VF-LD, PF-PL-PR-*H*-VF-LD
PF-YF	PL-PR, VF-LD, PF-PL-*H*-LD, PF-PR-*H*-VF, PL-*H*-YF-VF, PR-*H*-YF-LD, PF-PL-PR-YF-VF-LD
PF-VF	PL-*H*, YF-LD, PF-PL-PR-LD, PF-PR-*H*-YF, PL-PR-YF-VF, PR-*H*-VF-LD, PF-PL-*H*-YF-VF-LD
PF-LD	PR-*H*, YF-VF, PF-PL-PR-VF, PF-PL-*H*-YF, PL-PR-YF-LD, PL-*H*-VF-LD, PF-PR-*H*-YF-VF-LD
PL-LD	PR-VF, *H*-YF, PF-PL-PR-*H*, PF-PL-YF-VF, PF-PR-YF-LD, PF-*H*-VF-LD, PL-PR-*H*-YF-VF-LD
PF-PL-LD	PF-PR-VF, PF-*H*-YF, PL-PR-*H*, PL-YF-VF, PR-YF-LD, *H*-VF-LD, PF-PL-PR-*H*-YF-VF-LD

Also, since only one eighth of the full factorial was used, it is not possible to isolate the effects of factors and interactions. Even if it is assumed that the three and higher order interactions are less significant, the two-factor interaction effects still can not be directly obtained from the interaction section of Table 4 because a two-factor interaction is always confounded with some other two-factor interactions as shown in Table 5. However, under the assumption that three and higher order interactions are negligible and because the main effects are confounded only with three and higher order interactions (see Table 5), the effects of the two-factor interactions can be estimated by using the design matrix and the response values for each trial run given in Table 3, as outlined by Lochner and Matar (1990). Based on this technique, in the two cases where two-factor interactions proved to be significant, two-factor interaction tables and plots were constructed. However, in order to ascertain an exact quantitative understanding, some other method such as the response surface method (Box and Draper, 1987) has to be used, or a full factorial study has to be carried out.

It is noted at the outset that the results obtained here using a fractional factorial design were consistent (including the signs of the effects) with those obtained from the "one-at-a-time" study (Liu and Ritter, 1996). Therefore, no explanations of the causes of the effects are given here. The reader is referred to the detailed study by Liu and Ritter (1996).

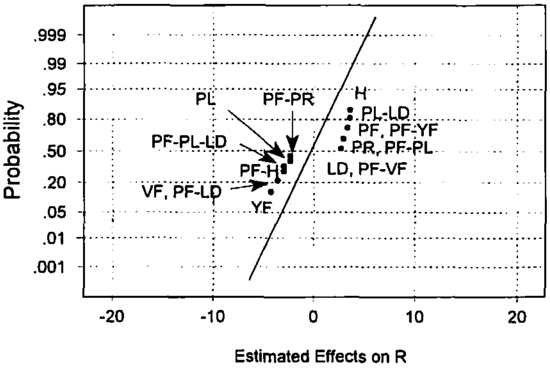

Figure 1. Normal probability plot for the estimated effects on the benzene vapor recovery, *R*.

Effects on Solvent Vapor Recovery (R)

The average benzene vapor recoveries at the low and high levels of factors or interactions for all runs are given in Table 4. The confounded effects of the factors and interactions are also presented in Table 4. Figure 1 displays the normal plot for these effects; note that some points overlap.

The average benzene vapor recovery (grand mean for *R*) was 97.86% (Table 3). According to Table 4, all effects of the factors or interactions on *R* were within the range of −4.274% (effect of YF) to 3.609% (effect of *H*). Compared to the average recovery of 97.863%,

Table 6. Two-factor interaction table for effects on solvent vapor recovery, R (%).

Interactions	Average R at different level combinations			
	(−, −)*	(−, +)*	(+, −)*	(+, +)*
PF-PL	98.81	93.52	99.24	99.88
PF-PR	93.52	98.81	99.24	99.88
PF-H	92.88	99.50	99.24	99.88
PF-YF	100.00	92.34	100.00	99.11
PF-VF	99.33	93.02	100.00	99.11
PF-LD	93.01	99.32	100.00	99.11
PL-PR	99.25	98.81	93.52	99.87
PL-H	98.58	99.47	93.54	99.86
PL-YF	100.00	98.05	100.00	93.40
PL-VF	99.34	98.71	99.98	93.41
PL-LD	99.47	98.58	93.54	99.86
PR-H	92.77	99.99	99.34	99.35
PR-YF	100.00	92.78	100.00	98.69
PR-VF	99.99	92.77	99.34	99.35
PR-LD	93.54	99.22	99.47	99.22
H-YF	100.00	92.11	100.00	99.34
H-VF	99.34	92.77	99.99	99.35
H-LD	93.54	98.58	99.47	99.86
YF-VF	100.00	100.00	99.32	92.12
YF-LD	100.00	100.00	93.01	98.44
VF-LD	99.99	99.33	93.01	99.11

*The first and second symbols correspond, respectively, to the levels of the first and second factors in the first column.

all of these effects were relatively small. These results were not surprising because the process was intentionally designed so that no significant solvent vapor breakthrough occurred during the adsorption step. However, once breakthrough occurs, all of these factors have significant effects on R (Liu and Ritter, 1996).

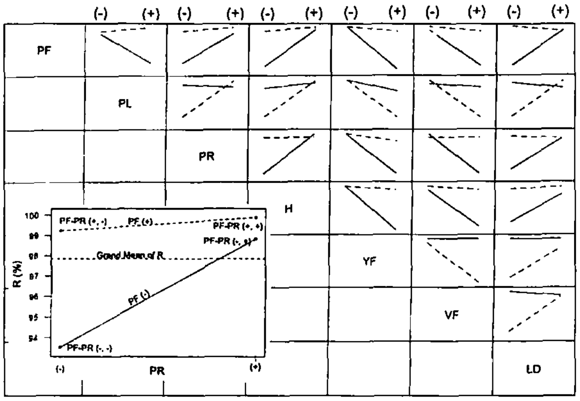

Figure 2. Two-factor interaction plots for the effects on benzene vapor recovery, R. Solid lines represent low levels (-) of the factors to their left; dotted lines represent high levels (+) of the factors to their left; left ends of the lines in each plot represent the low level of the factor underneath; right ends of the lines in each plot represent the high level of the factor underneath (see insert).

It is seen from the normal plot (Fig. 1) that no single straight line can cross all the points representing these effects. This indicated that although the effects of these factors and interactions were relatively small, interaction effects did exist on the solvent vapor recovery. Note that once a factor is involved in an interaction, its effect can not be interpreted alone according to its main effect; and the effect of this factor has to be analyzed according to the interaction. Therefore, two-factor interaction tables and plots were constructed (Lochner and Matar, 1990); the results are displayed in Table 6 and Fig. 2. The slopes of the two straight lines of each interaction plot in Fig. 2 were quite different, indicating marked two-factor interaction effects existed on R. However, the absolute magnitudes of these interaction effects can be judged only from the results given in Table 6, because the axis scales of each interaction plot in Fig. 2 are generally different. To show how to interpret these effects, the PF-PR interaction is used; refer to the insert in Fig. 2.

When the PSA-SVR process was operated at the high level of the PF (the dotted line in the interaction plot), increasing the PR from its low to high level (moving from left to right), improved the R from 99.24% to 99.88%; when this process was operated at the low level of the PF (the solid line in the interaction plot), increasing the PR from its low to high level improved the R from 93.52% to 98.81%, a much bigger improvement compared to that at the high level of PF. Similarly, when the process was operated at the low level of PR (left ends of the straight lines in the interaction plot), increasing PF from its low to high level improved R from 93.52% to 99.24%; when this process was operated at the high level of PR (the right ends of the two straight lines in the interaction plot), increasing the PF from its low to high level improved R from 98.81% to 99.88%, a much smaller improvement compared to that at the low level of PR. Moreover, operating the PSA process at a higher PF (dotted line in the interaction plot) or a higher PR (right ends of the two straight lines) always improved the solvent vapor recovery. The interpretation of all the other two-factor interactions can be done in the same way. Generally, when the PSA process was operated in each case at a higher PF, PR, H and LD, or a lower PL, YF and VF, R improved; and, in each case, changing any of the other six factors had less effects on R than they did at the opposite level of the factor in question.

Effects on Solvent Vapor Enrichment (E) and Relative Enrichment (E_R)

The individual and average benzene vapor enrichments and relative enrichments for all sixteen runs are given in Table 3. The effects of all the confounded factors and interactions are given in Table 4. Figures 3 and 4 display the normal plots for the effects on E and E_R, respectively.

From the normal plots, it is seen that all points that represented the effects fell approximately on a straight line, except for the confounded effects of the PF, YF and PR. Since all the confounded interaction effects were negligible (which necessarily implied that the interactions involved in the alias were quite small), it was reasonable to consider that the effect given in Table 4 for each factor was the main effect of that factor. It is also seen from Table 4 that changing PF and YF from their low to high levels had a negative effect on E, while changing PR from its low to high level had a positive effect on E. These same trends can be seen from the normal plot (Fig. 3) in which the points representing the effects of PF and YF were to the left of the straight line, while the point representing the effect of PR was to the right hand of the straight line. For example, increasing PF from 1.5 to 2 (an increase of 33.3%) decreased E from 7.744 to 6.534 (a decrease of 15.6%). Similarly, increasing YF from 2.5 to 5.0% (100% increase) decreased E from 8.322 to 5.956 (a decrease of 28.4%). On the other hand, increasing PR from 20 to 30 (50% increase) increased E from 6.353 to 7.925 (an increase of 24.7%).

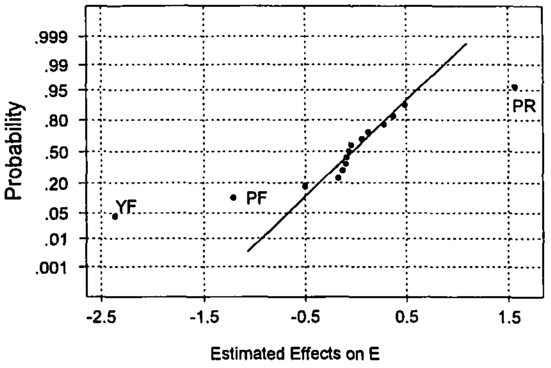

Figure 3. Normal probability plot for the estimated effects on the benzene vapor enrichment, E.

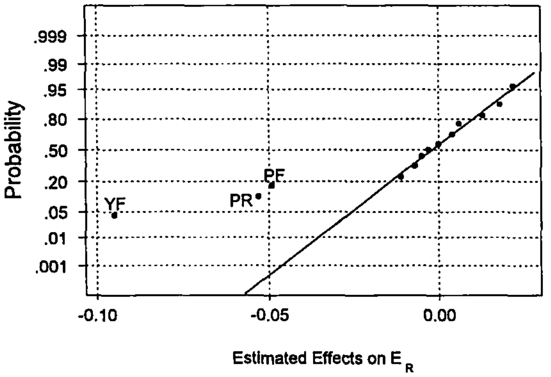

Figure 4. Normal probability plot for the estimated effects on the relative benzene vapor enrichment, E_R.

It is interesting to note that all three factors (PF, PR, YF) had negative effects on E_R, whereas the PR had a positive effect on E. This implied that although increasing PR increased the absolute solvent vapor enrichment, operating the PSA-SVR process at a higher PR caused the PSA-SVR process to deviate more from the most idealized conditions. In fact, the average E_R for all sixteen runs was only 0.291, much lower than that for the idealized case, which is unity. The small E_R verified the importance of the effects of non-idealities on the PSA-SVR process performance, as discussed in detail by Liu and Ritter (1996). It also indicated that there may be much room for optimizing these process conditions.

Effects on Light Product Purity (y_p)

The individual and average light product purities for all 16 runs are given in Table 3. Table 4 displays the effects of all the confounded factors and interactions on y_p. The normal plot is displayed in Fig. 5; note that some points overlap.

The magnitudes of the effects of the factors and interactions (Table 4) and the normal plot (Fig. 5) show that all factors and interactions had significant effects on y_p, at least with respect to restrictions imposed by environmental regulations. Thus, two-factor interaction tables and plots were constructed (Lochner and Matar, 1990); the results are given in Table 7 and Fig. 6. Again, for

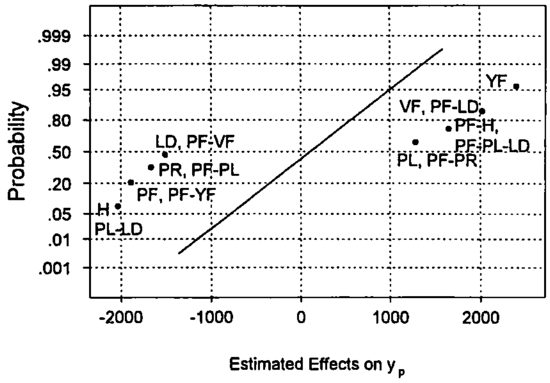

Figure 5. Normal probability plot for the estimated effects on the light product mole fraction, y_p.

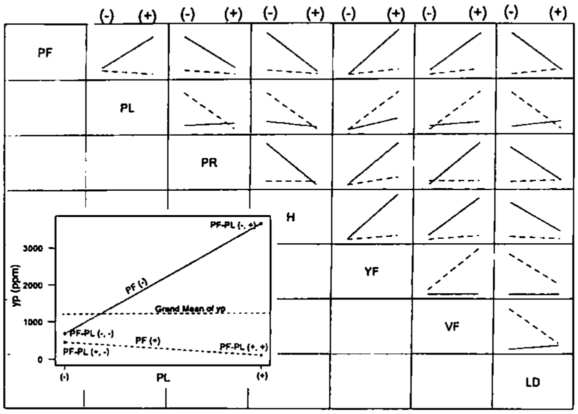

Figure 6. Two-factor interaction plots for the effects on light product purity, y_p. Solid lines represent low levels (-) of the factors to their left; dotted lines represent high levels (+) of the factors to their left; left ends of the lines in each plot represent the low level of the factor underneath; right ends of the lines in each plot represent the high level of the factor underneath (see insert).

instructive purposes, the PF-PL interaction effects are used; refer to the insert of Fig. 6.

Table 4 shows that operating the PSA-SVR process at a higher PF caused y_p to decrease. At a PF of 2, the average y_p was 260 ppm, while at a PF of 1.5, the average y_p was 2148 ppm. Moreover, according to the interaction tables and plots, at a lower level of PF compared to a higher one, it was easier to increase y_p when changing the other six factors in the direction of increasing y_p. Similarly, when a higher PL was used compared to a lower one, it increased y_p (Table 4), and when changing the other factors in the direction of increasing y_p, it made it easier to increase y_p. Similar conclusions can be drawn for all the two-factor interactions given in Table 7 and Fig. 6. Generally, when the PSA-SVR process was operated in each case at a higher PR, PF, H and LD, or a lower PL, YF and VF, y_p decreased and, in each case, changing any of the other six factors had less effects on y_p than they did at the opposite level of the factor in question.

Table 7. Two-factor interaction table for effects on light product purity, y_p (ppm).

	Average y_p at different level combinations			
Interactions	(−, −)*	(−, +)*	(+, −)*	(+, +)*
PF-PL	671.98	3625.77	448.28	73.03
PF-PR	3625.24	672.01	448.28	73.03
PF-*H*	3991.63	305.62	448.76	72.55
PF-YF	0.03	4297.22	0.00	521.31
PF-VF	383.84	3913.41	0.48	520.83
PF-LD	3913.38	383.87	0.48	520.83
PL-PR	3625.24	672.01	448.28	73.03
PL-*H*	823.38	296.88	3617.01	81.29
PL-YF	0.00	1120.25	0.03	3698.27
PL-VF	375.1	745.15	9.22	3689.08
PL-LD	296.88	823.38	9.22	3616.98
PR-*H*	4064.78	8.74	375.61	369.43
PR-YF	0.00	4073.52	0.03	745.01
PR-VF	8.74	4064.78	375.58	369.46
PR-LD	3616.50	457.02	297.36	447.68
H-YF	0.03	4440.36	0.00	378.17
H-VF	375.58	4064.81	8.74	369.43
H-LD	3616.98	823.41	296.88	81.29
YF-VF	0.00	0.03	384.32	4434.20
YF-LD	0.00	0.03	3913.86	904.67
VF-LD	0.48	383.84	3913.38	520.86

*The first and second symbols correspond, respectively, to the levels of the first and second factors in the first column.

Effects on Bed Utilization (BCF)

The portion of the used bed was represented by the BCF. The average BCF for all sixteen runs is given in Table 3. The effects of the confounded factors and interactions are given in Table 4. Figure 7 displays the normal plot.

The results in Table 4 show that the second and higher order confounded interaction effects, except for two cases, caused the absolute value of the BCF to change by less than 5%. This indicated that it was

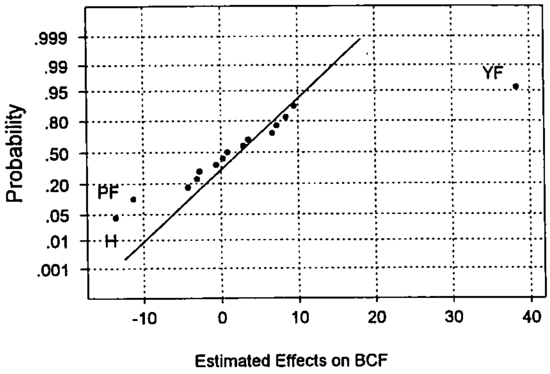

Figure 7. Normal probability plot for the estimated effects on the bed capacity factor, BCF.

reasonable to use the effect of each factor given in Table 4 to approximate the main effect of that factor, i.e., confounded effects were negligible. Moreover, in some cases the effect of the factor on the BCF was quite large, ranging from 38.32% for YF to -13.53% for H; and only two of the factors changed the absolute value of the BCF by less than 5% (PL and LD).

The normal plot also showed that only the PF, H and YF had significant effects on the BCF. Remember, if the amount of solvent vapor fed into the bed was fixed, a larger BCF indicated a higher probability of solvent vapor breakthrough during the adsorption step, and thus a poorer process performance. Increasing PF from 1.5 to 2.0 (an increase of 33.3%) decreased the BCF from 84.214% to 72.945% (a decrease of 13.38%). The effect of H on the BCF was even more marked. Decreasing H from 0.02092 to 0.004184 kJ/(m^2 s K) (a decrease of 80%) increased the BCF from 71.814% to 85.345% (an increase of 18.84%). However, YF had the largest effect on the BCF. Increasing YF from 2.5 to 5.0% (100% increase) increased the BCF from 54.419% to 97.739% (an increase of 79.6%). Also, increasing the PL, PR and VF all increased the BCF, but their effects were less significant. LD had essentially no effect on the BCF (its effect was only 0.302%), indicating that the PSA-SVR process was operated very close to equilibrium.

Significance of Results

What do all of these results mean, and why is this fractional factorial design approach better than the more traditional and user-friendly one-at-a-time approach? One likes to operate a PSA process at the optimum operating conditions and also where the effects of disturbances are a minimum. Clearly, factor interactions affect both the optimization and the sensitivity of a process because if they exist, the performance of the process depends on the particular factor level combination employed. It is impossible to determine factor interactions using the one-at-a-time approach, at least without performing numerous runs at all possible factor levels and combinations. Even then the interpretation may be questionable.

This fractional factorial design study of a PSA-SVR process showed that some significant factor interactions do exist, and that they have a marked effect of the process performance. Other results showed that no significant factor interactions exist for some process parameters, which lends credence to some of the results obtained from the one-at-a-time approach. However, what is truly exciting about these results is that only 16 runs were required to obtain a significant amount of information on how seven factors (parameters) and their interactions affected the performance of a PSA-SVR process. This is in contrast to the 128 runs required for a full factorial design and an unknown number of runs for the one-at-a-time approach. Nevertheless, the one-at-a-time approach is still very useful because it generally gives a very clear picture of what causes the particular effect in question, as demonstrated by Liu and Ritter (1996).

Conclusion

A 2^{7-3} fractional factorial study was carried out by computer simulation on the periodic state performance of a PSA-SVR process. Only 16 simulation runs were made to study the effects of seven factors (PF, PR, PL, YF, VF, H and LD) and their interactions on the process performance, which was measured in terms of R, E, E_R, y_p and BCF. The emphasis of this parametric study was placed on ascertaining the effects of two-factor and higher order interactions on the process performance. This kind of information is impossible to obtain with the more familiar one-at-a-time approach that is frequently used in parametric studies.

The following conclusions were drawn from the results: Two-factor interaction effects existed on R, although all of these effects were relatively small under the conditions investigated. Nevertheless, it was observed that R improved when the PSA process was operated in each case at a higher PF, PR, H and LD, or a lower PL, YF and VF; and, in each case, changing any of the other six factors had less effects on R than they did at the opposite level of the factor in question. No significant two-factor and higher order interaction effects existed on E and E_R. Only the PF, PR and YF had the most significant effects on E and E_R. Increasing PF and YF decreased E and E_R, whereas increasing PR increased E, but decreased E_R, indicating that operating the PSA-SVR process at a higher PR made the process deviate farther from the most idealized conditions. Strong two-factor interaction effects were found on y_p. The results showed that when the PSA-SVR process was operated in each case at a higher PR, PF, H and LD, or a lower PL, YF and VF, y_p decreased and, in each case, changing any of the other six factors had less effects on y_p than they did at the opposite level of the factor in question. There were no significant two-factor and higher order interaction effects observed on BCF. Only YF, PF and H had significant effects on BCF. Interestingly, LD had almost no effect on BCF in this PSA-SVR process, indicating that local equilibrium conditions dominated even though realistic mass and heat transfer effects were included in the model.

Overall, this study demonstrated the usefulness of fractional factorial design in the study of PSA processes. It revealed, for the first time, that significant two-factor interactions exist and have a marked effect on the PSA process performance, i.e., the effect of one factor involved in an interaction depends on the level of the other factor. These two-factor interactions must be accounted for when optimizing a PSA process to operate at peak performance while minimizing disturbances. However, it should be pointed out that the quantitative results obtained from this design apply only to the conditions under which they were obtained. If these conditions are changed, e.g., by changing the factor levels, the results may be different.

Nomenclature

BCF	bed capacity factor, %
b, b_0	isotherm parameters, $m^3/(mol\ K^{0.5})$
C_{pg}	gas phase heat capacity, kJ/(kg K)
C_{ps}	solid phase heat capacity, kJ/(kg K)
E	enrichment
E_I	ideal enrichment
E_R	relative enrichment
H	heat transfer coefficient, $kJ/(m^2\ s\ K)$
ΔH	heat of adsorption, kJ/mol
k	number of factors, or mass transfer coefficient, 1/s
l	number of levels
L	bed length, m
LD	bed length to diameter ratio
PF	purge to feed ratio
P_H	adsorption high pressure, kPa
P_L	desorption pressure, kPa
PL	pressure level, represented by P_L
PR	pressure ratio
q	amount adsorbed, mol/kg
q^*	equilibrium amount adsorbed, mol/kg
q_f^*	equilibrium amount adsorbed at the feed conditions, mol/kg
r_b	bed radius, m
R	solvent vapor recovery, %; or gas constant, m^3 (mole K)
T	temperature, K
T_0	ambient temperature, K
t	time, s
u	interstitial velocity, m/s
VF	volumetric feed flow rate, m^3 STP/s
YF	feed mole fraction
y_p	light product mole fraction
z	axial coordinate, m

Greek Symbols

ρ_g	gas phase density, kg/m^3
ρ_s	solid phase density, kg/m^3
ε	bed void fraction

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