Energy of Vented Gases as a Means for Improving Product Purity during Swing Adsorption

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Abstract—The equilibrium swing adsorption model is used to show that the purity of the product gas linearly increases with decreasing the ratio of the gas pressure during the recovery stage to the gas pressure during the adsorption step. We propose to use the energy of the vented gas for decreasing this ratio through ejecting the vented gas flow. A fundamentally new swing adsorption flowsheet with a gas ejector is proposed.

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A common distinctive feature of swing adsorption, despite the variety of its implementations, is the difference between the pressure at which selective adsorption (i.e., the separation of the gas components) occurs and the pressure at which the remaining component is vented, which leads to the recovery of the adsorbent [1]. The underling idea of the method is a thermodynamic cycle whose major stages are the selective adsorption of one gas component, which occurs at pressure p_a , and the recovery of the adsorbate bed, which is implemented through venting this gas component at lower pressure p_0 [1, 2]. Due to the small time lag of gas venting, swing adsorption has been widely used in technology [3, 4]. A weakness of swing adsorption is a relative low purity of the product gas. For example, for oxygen production from air in advanced swing adsorption setups, the product gas as a rule contains at least 2.5% nitrogen; an extra swing adsorption setup is required in order to improve the purity of the product gas, which decreases the efficiency of the cycle. It is of interest to study swing adsorption flowsheets that would improve product purity without significant energy consumption.

EFFECT OF THE PRESSURE RATIO ON PRODUCT PURITY

The main stages of pressure swing adsorption are adsorption, desorption, and adsorber filling with the product gas; sometimes, the swing adsorption flowsheet is supplemented with adsorbent purging with the product gas [1]. The feed gas at the adsorption stage enters the adsorber, which is initially filled with the product gas to pressure p_0 . Adsorption occurs at a virtually constant pressure p_0 ; a sharp and stationary adsorption interface is formed with width $l \ll L$, where L is the adsorber length. The effect of construction and process parameters on interface length and the convective instability of the interface were studied in [5, 6]. Entropy production near the adsorption interface was studied in [7, 8].

The adsorption interface divides the adsorber volume into two parts. In front of the interface, the gas composition corresponds to the composition of the product gas; behind the interface, the gas composition coincides with the composition of the feed gas. Therefore, at the end of the adsorption stage, the partial pressure of the *i*th component $(i = 1 \text{ or } 2)$ in the gas phase is $p_0 = RTc_{0i}$, where $R = 8.314$ kJ/(mol K), *T* is temperature (K) , and c_{0i} is the molar concentration of the *i*th component $(i = 1 \text{ or } 2)$ in the feed gas. The total gas pressure in the adsorber during the adsorption stage is $p_0 = p_{01} + p_{02}$. Gas venting is carried out at pressure p_1 , which is lower than p_0 . An important parameter of swing adsorption is the ratio

$$
\alpha = \frac{p_1}{p_0} < 1.
$$

Let us consider an isothermal process in order to find the $\beta(\alpha)$ function, where β is the mole fraction of the first (impurity) component in the product gas. Let us determine c_{1i} , the molar concentration of the *i*th component in the gas phase of the adsorber of volume V_0 after the gas-vent stage is over, on the assumption that the adsorbent is in equilibrium with the gas discharged from the adsorber to the external volume V_1 at pressure p_1 . For linear adsorption, we can write the mass balance for the *i*th component:

$$
(\varepsilon + \chi_i(1-\varepsilon))V_0C_{0i} = (\varepsilon + \chi_i(1-\varepsilon))V_0c_{1i} + V_1c_{1i'}
$$

$$
i = 1, 2.
$$

Here, ε is the bed porosity and χ _{*i*} is the Henry constant for the *i*th component.

By definition, α can be represented as

$$
\frac{c_{11} + c_{12}}{c_{01} + c_{02}} = \alpha.
$$
 (2)

Solving the linear set of algebraic equations (1) – (2) for c_{11} , c_{12} , and V_1 , we obtain

$$
c_{11} = \frac{c_{01}}{2}d\left(1 - \sqrt{1 - \frac{4\alpha}{\gamma(1 - k)d^2}}\right),
$$

\n
$$
c_{12} = \frac{\alpha c_{01}}{\gamma} - c_{11},
$$
\n(3)

where $d = 1 + \frac{k}{\gamma(1-k)} + \frac{\alpha}{\gamma}, k = \frac{k_2}{k_1}, k_i = \varepsilon + \chi_i(1-\varepsilon),$ $\frac{k_2}{k_1}$

 $\gamma = \frac{c_{01}}{c_{01}}$. $\frac{c_{01}}{c_{01} + c_{02}}$

The number of moles of the *i*th component that will be in the adsorber after the gas-vent stage is over, m_{1i} , can be represented as $m_{1i} = V_0 k_i c_{1i}$. When $\alpha \ll 1$, after linearizing relationships (3) for α , we obtain

$$
m_{11} = \frac{V_0 c_{01} k_1 \alpha}{\gamma (1 - k) + k}, \quad m_{12} = \frac{V_0 c_{01} k_1 k^2 (1 - \gamma) \alpha}{\gamma (\gamma (1 - k) + k)}.
$$
 (4)

During the filling of the adsorber to the starting pressure p_0 , *M* moles of the product gas are fed to the adsorber with the mole fraction of the impurity component equal to β. Denoting by m_{2i} the number of moles of the *i*th component contained in the adsorber after the filling stage is over, we can write

$$
m_{2i} = m_{11} + \beta M, \quad m_{22} = m_{12} + (1 - \beta)M.
$$

On the other hand, $m_{2i} = k_i c_{2i} V_0$, where c_{2i} is the molar concentration of the *i*th component in the gas phase of the adsorber after the filling stage is over.

Two equations should be made for β and *M*. One equation is the consequence of the constraint that the pressure after the filling stage is equal to the pressure of the feed gas that enters the adsorber during the adsorption stage; i.e., $c_{21} + c_{22} = c_{01} + c_{02}$, which can be represented, using Eq. (4), as

$$
\frac{(\gamma + (1 - \gamma))\alpha}{\gamma(\gamma(1 - k) + k)} + x\left(\beta + \frac{1 - \beta}{k}\right) = \frac{1}{\gamma}
$$
 (5)

with $x = M/(k_1 V_0 c_{01})$. The other equation is the consequence of the constraint that the gas composition after the filling stage coincides with the composition of the product gas; i.e., $c_{21} = \beta(c_{01} + c_{02})$, which can be represented as

$$
\frac{\alpha}{\gamma(1-k)+k} + \beta x = \frac{\beta}{\gamma}.
$$
 (6)

For the case at hand with low α and β, from Eqs. (5) and (6) we finally arrive at

$$
\beta = \frac{\alpha \gamma}{(1-k)(k+\gamma(1-k))}.
$$
 (7)

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One can see that β, i.e., the impurity level of the product gas, linearly decreases with decreasing α . When the gases to be separated have similar adsorption properties $(k \approx 1)$, the interface thickness increases [6]; in order to achieve the required purity level, in addition to decreasing α, one should increase the adsorber length to make the interface sufficiently thin in relative units.

In practice, the impurity level of the product gas is lower than that calculated from Eq. (7). This is because of the nonuniform distribution of the impurity gas along the adsorbent length during the filling stage. At the initial adsorption stage, therefore, the purity of the product gas is higher than the average; as a result, the earlier entrance to the adsorption stage improves product purity. However, the active volume of the adsorber decreases and the efficiency drops. Purging the adsorber with the product gas also slightly improves product purity, but the output decreases at the same time. Thus, relationship (7) can be considered as the upper estimate of the impurity of the product.

SWING ADSORPTION FLOWSHEET WITH A GAS EJECTOR

The use of vacuum pumps to decrease the pressure during the gas-vent stage in swing adsorption flowsheets [9] increases energy consumption. The energy of the vented gas flow can be used to decrease α as follows: the vented gas flow is directed to a gas ejector, which will decrease the pressure during the gas-vent stage when connected to the adsorber. The figure demonstrates a swing adsorption flowsheet with three adsorbers and an ejector provided that $p_0 > 2$ at. With the use of a subsonic ejector, its inlet pressure is 2 at [10]. The gas-vent stage is implemented in three steps. In the beginning of the gas-vent stage (at pressures of $2 < p < p_0$ at), the vented gas is directed to a storage (a gas collector) with a pressure of about 2 at. The collector is the gas source for the ejector. In the middle of the gas-vent stage (at pressures of $1 < p < 2$ at), the gas is discharged to the ambiance passing by the ejector line. Finally (when $p < 1$ at), the adsorber is connected to the ejector, which creates vacuum on the order of 10⁻² at, thus decreasing α to ~10⁻³ and decreasing the product impurity level β to \sim 10⁻².

In the flowsheet for adsorber recovery during swing adsorption shown in the figure, the gas is vented from the end of the adsorber. The recovery time with this gas vent organization can appear unacceptably long because of a significant hydraulic drag of the bed along the adsorber axis. Gas venting through the lateral surface of the adsorber can shorten this time. The choice of the gas-vent organization is dictated by the required length of the recovery stage, which should correlate with the length of the working swing adsorption cycle. In the approximation of a semiinfinite adsorber, the following relationship was derived for the recovery time

Three-step flowsheet of the recovery stage: (1) partial gas venting to gas collector *C* to acquire the pressure equal to the pressure in the collector (2 at), (2) gas venting to the atmosphere (to the atmospheric pressure), and (3) gas venting at a low pressure created by the ejector, which is fed by the gas from the collector. Notation: *A*1, *A*2, and *A*3 are adsorbers.

as a function of the process and construction parameters of swing adsorption [11]:

$$
t_L = 45.3 \left(\frac{1+\alpha}{1-\alpha}\right)^2 \frac{\left(1-\epsilon\right)^2 \chi \mu L^2}{\epsilon^3} \left[\frac{p}{\Delta p} \right]^2 - \left(\frac{p_0}{\Delta p}\right)^2 \right]^{-2} . (8)
$$

Here, t_L is the time during which the pressure in the cross section of the adsorbent bed separated by distance *L* from the outlet cross section will decrease to a certain value p , ε is the bed porosity, d_p is the particle diameter, and ∆*p* is the difference between the pressure in the beginning of the recovery stage and the ambient pressure. The *L* value is affected by the gas-vent organization: when the gas is vented through the end cross section, *L* approaches one-half length of the adsorbent bed; when the gas is vented through the lateral surface of the adsorber, *L* approaches the bed radius.

CONCLUSIONS

(1) An equilibrium model as applied to swing adsorption showed that the purity of the product gas improves linearly with decreasing pressure at the recovery stage.

(2) In order to decrease the pressure at the recovery stage, it is advisable to implement this stage in three steps. To decrease the pressure at the third step of the recovery stage, the discharge gas flow is fed to a gas ejector. A swing adsorption flowsheet with an ejector is proposed.

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