Design and simulation of VPSA separation process for VOCs removal

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Abstract

Vacuum pressure swing adsorption (VPSA) model for volatile organic compounds (VOCs) system was proposed and simulated by ASPEN ADSIM software. The dynamic results of the gas composition in the column, the outlet gas concentration, and the adsorption column were obtained, which presented the gaseous phase change in the whole separation process. With detailed physical parameters, the model could simulate and predict the actual VPSA separation process.

Introduction

Accumulation of volatile organic compounds (VOCs) in the human body and environment has become a subject of discussion even if very low concentration since VOC emission is one of the major sources of air pollution. Pressure swing adsorption(PSA) has been widely utilized for purification and separation of gases by developing various kinds of processes. PSA process has been applied to solvent elimination and its demand has increased from viewpoints of compact apparatus, economical energy and so on. To separate and recover very low concentration organic vapor we propose here a new PSA process using ASPEN ADSIM. The purpose of this paper is to theoretically analyze the removal of VOC by means of VPSA process.

Process description

VPSA is a cyclic process where some components from a multi-component gas mixture are selectively retained in a porous material. A schematic diagram of cyclic VPSA process considered in the paper is presented in Figure 1. Before breakthrough of these components, the column must be regenerated. Regeneration is carried out by reducing the total pressure of the system under a pre-defined scheduling. The regeneration steps will define the final power consumption of the process. The selective adsorption of these components is normally carried out at the highest pressure of the system and then its desorption (regeneration) is accomplished at a lower pressure, involving use of vacuum. In the case of removing VOCs from oil mist, VOCs will be one of the most adsorbed gases and the scheduling of the VPSA technology should be based on this phenomenon.

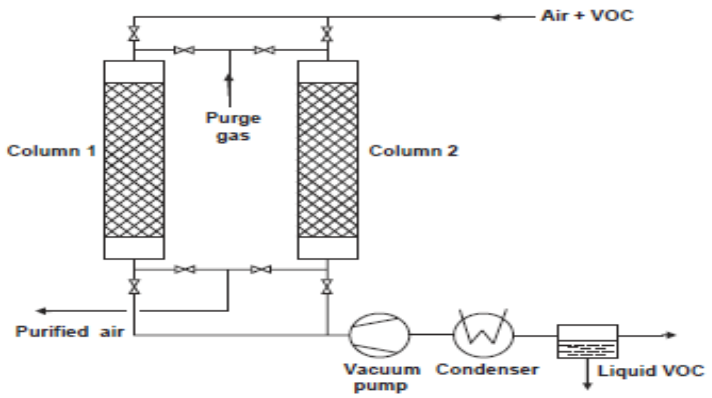

Figure 1. A schematic diagram of the 2-bed VPSA process

Feed component and simulation process

The main components are shown in Table 1 and simulation process is shown in Figure 2.

Table 1. Feed components used in simulation

NO.	components	molecular formula	symbol	contents (wt%)
1	nitrogen	N2	N2	92
2	benzene	C_2H_6	BZ	5.5
3	*m*-xylene	C_8H_{10}	M-XYL	2.5

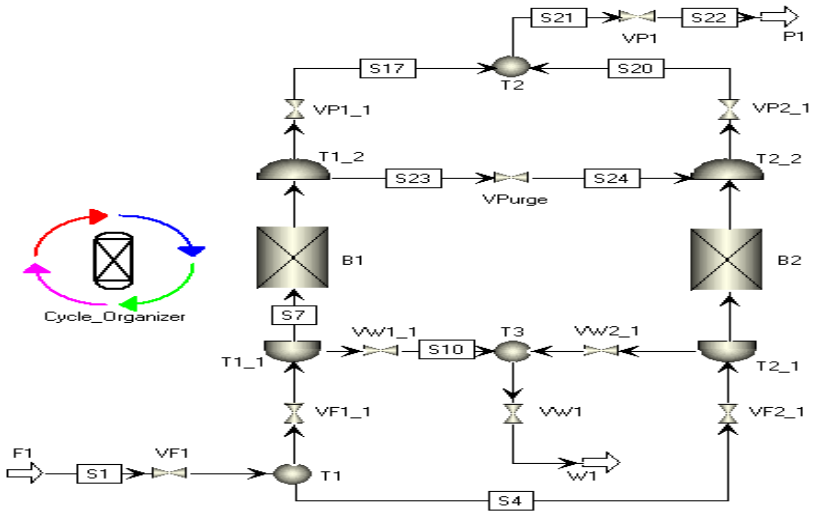

Figure2. Aspen adsorption VPSA process simulation flowsheet

Mathematical models and parameters

The assumptions the model equations are:

·Continuity equation:

$$\varepsilon_i E_{Z_i}\frac{\partial c_i}{\partial z^2}-\varepsilon E_{ri}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_i}{\partial r}\right)+\frac{\partial(v_g c_i)}{\partial z}+\varepsilon_B\frac{\partial c_i}{\partial t}+j_i=0$$

Where, ε_i-bed porosity, E-diffusivity coefficient, r-bed radius, ε_B-total of bed and pellet porosity, v_g-space velocity, j_i-mass transfer rate

·Ergun equation:

$$\frac{\partial p}{\partial z}=\left(\frac{1.5\times10^{-3}(1-\varepsilon_i)^2}{(2r_p\Psi)^2\varepsilon_i^3}\mu v_g+1.75\times10^{-5}M\rho_g\frac{(1-\varepsilon_i)}{2r_p\Psi\varepsilon_i^3}v_g^2\right)$$

Where, μ-viscosity, M-molecular weight, Ψ-adsorbent sharp factor, r_p-pellet radius

·The resistances to mass transfer equation:

$$j_i=MTC_i(c_b-c_s)=-\rho_s\frac{\partial w_i}{\partial t}$$

Where, j_i-mass transfer rate, MTC_i-mass transfer coefficient, C_i-gas concentration, C_i-gas-solid interfacial concentration, C_s-solid concentration, ρ_s-bulk solid density of adsorbent

·Langmuir model equation:

$$w_i=\frac{IP_1P_i}{1+IP_2P_i}$$

Where,IP_1/IP_2 -parameters of isotherms, P_i-adsorption pressure,ω_i -adsorption weight

Model parameters used in simulation are listed in Table 2.

Table 2. Model parameters used in simulation

Variables	Values	Units	Description
Hb	350	mm	Height of adsorbent layer
Ib	35	mm	Internal diameter of adsorbent layer
Ei	0.32	$m^3 void/m^3 bed$	Inter-particle voidage
Ep	0.26	$m^3 void/m^3 bed$	Inter-particle voidage
RHOs	730	kg/m^3	Bulk solid density of adsorbent
Rp	1	mm	Adsorbent particle radius
SFac	1.0		Adsorbent shape factor
MTC("Nitrogen")	0.00761	s^{-1}	Constant mass transfer coefficients
MTC("Oxygen")	0.04476	s^{-1}	Constant mass transfer coefficients
MTC("Benzene")	21	s^{-1}	Constant mass transfer coefficients
MTC("M-xylene")	17.4	s^{-1}	Constant mass transfer coefficients
IP(1,"Nitrogen")	0.00901	$Kmol \cdot kg^{-1} \cdot bar^{-1}$	Isotherm parameter
IP(1,"Benzene")	0.57	$Kmol \cdot kg^{-1} \cdot bar^{-1}$	Isotherm parameter
IP(1,"M-xylene")	0.39	$Kmol \cdot kg^{-1} \cdot bar^{-1}$	Isotherm parameter
IP(1,"Oxygen")	0.00936	$Kmol \cdot kg^{-1} \cdot bar^{-1}$	Isotherm parameter
IP(2,"Nitrogen")	3.3712	$Kmol \cdot kg^{-1} \cdot bar^{-1}$	Isotherm parameter
IP(2,"Benzene")	403.41	$Kmol \cdot kg^{-1} \cdot bar^{-1}$	Isotherm parameter
IP(2,"M-xylene")	356.73	$Kmol \cdot kg^{-1} \cdot bar^{-1}$	Isotherm parameter
IP(2,"Oxygen")	3.5038	$Kmol \cdot kg^{-1} \cdot bar^{-1}$	Isotherm parameter

Results and conclusion

The present study was undertaken as a step towards the development of strategy for simulation based on design and simulation of VPSA process for VOCs removal.

Figure 3 shows the adsorption isotherms of benzene. It was fitted according to Langmuir model.

On the basis of the above mathematical models and parameters, we simulate adsorption-desorption cycles. Figure 4 shows the concentration curves of benzene and m-xylene during cycles. The concentration in adsorption tower reaches a steady state after the second cycle.

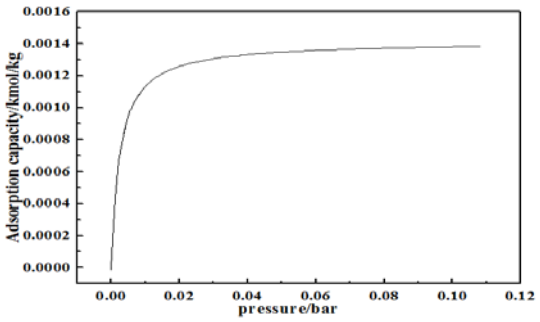

Figure 3. Adsorption isotherms of benzene

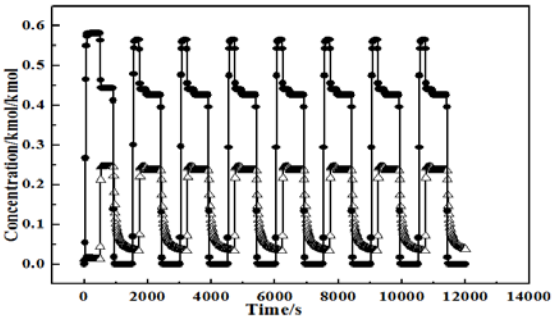

Figure 4. Concentration curves of benzene and m-xylene among cycles

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