A Novel Technique to Solve Mathematical Model of Pressure Swing Adsorption System for Oxygen Separation from Air

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Abstract— The mathematical modeling of a Pressure Swing Adsorption (PSA) system is discussed in detail for the Skarstrom cycle of two-bed process. The system is used to get pure oxygen product from the air with the use of zeolite 13X as an adsorbent. There are complex partial differential equations (pdes) which may not solve by analytical methods. There is no provision for solving it in any other software other than Matlab. All the equations are rearranged and written into dimensionless quantities, to make it easier. It is a novel technique of solving these complex pdes. After that we have converted these pdes into ODEs (Ordinary Differential Equations) by using OCFE (Orthogonal Collocation on Finite Elements) method. Now, these ODEs can be solved using different solvers like ode23, ode45, ode113, ode15s, ode23s, ode23t, ode23tb. The results obtained by this model will be compared to real industrial data.

I. INTRODUCTION

Pressure Swing Adsorption (PSA) is a common process technique for purification of gas and for the separation of gas mixtures. A large variety of binary and multi component gas mixtures are commercially separated using this technology. This extraordinary process has been possible due to the development of tailor-made adsorbents for given separations and various sophisticated cycles employing multiple beds which improve the performance of the process. The adsorption plants consist of several fixed-bed absorbers and are operated as cyclic multistep processes; the most common is via cryogenic distillation. There is no provision for solving it in any other software other than Matlab. All the equations are rearranged and written into dimensionless quantities, to make it easier. It is a novel technique of solving these complex pdes. After that we have converted these pdes into ODEs (Ordinary Differential Equations) by using OCFE (Orthogonal Collocation on Finite Elements) method. Now, these ODEs can be solved using different solvers like ode23, ode45, ode113, ode15s, ode23s, ode23t, ode23tb. The results obtained by this model will be compared to real industrial data.

II. AIR SEPARATION

An air separation plant separates atmospheric air into its primary components, typically nitrogen and oxygen; and sometimes also argon and other rare inert gases. There are various technologies that are used for the separation processes; the most common is via cryogenic distillation.

A. Cryogenic Distillation Process:

This process was pioneered by Dr. Carl von Linde in the early 20th century and is still used today to produce high purity gases. The cryogenic separation process requires a very tight integration of heat exchangers and separation columns to obtain a good efficiency and all the energy for refrigeration is provided by the compression of the air at the inlet of the unit. In addition to the cryogenic distillation method there are other methods such as Membrane, Pressure Swing Adsorption (PSA), and Vacuum Pressure Swing Adsorption (VPSA), which are typically used to separate a single component from ordinary air. Production of high purity oxygen, nitrogen, and argon which are used for Semiconductor device fabrication requires cryogenic distillation, though. Similarly, the only viable sources of the rare gases like neon, krypton, and xenon are the distillation of air using at least two distillation columns. Cryogenic ASUs are built to provide nitrogen and/or oxygen and often co-produce argon where liquid products (Liquid nitrogen “LIN”, Liquid oxygen “LOX”, and Liquid argon “LAR”) can only be produced if sufficient refrigeration is provided for in the design.

B. PSA Process:

After compacted and purified to remove oil, water and dust, environmental air will enter the pressure swing adsorption device composed by 2 adsorption towers (up to a few ppm). Since the freezing points of H2O and CO2 are well above the cryogenic temperatures of liquefied air, there is a distinct possibility of occluding the distillation column internals if the air is supplied to the cryogenic distillation unit in its crude form [10]. Besides, owing to the insolubility of hydrocarbons in liquid oxygen, there is a danger of their accumulation in the reboiler of the distillation column thus posing an explosion hazard. In case of noncryogenic processes such as pressure swing adsorption, impurities such as water vapor and carbon dioxide are found to adsorb strongly, and to some extent, irreversibly on the adsorbents used for the separation of air.
equipped with carbon molecular sieve. The compressed air flow from bottom to top, the nitrogen will be adsorbed by adsorbents like 13X, 10X, 4A, 5A, LiX, LiLSX, LiAgX etc., and oxygen will flow out from top adsorption tower and enter the raw oxygen buffer tank. After a period of time, the adsorbent will be saturated by nitrogen adsorbed, which needs to be regenerated. The regeneration will be achieved by stopping adsorption and decreasing the pressure of adsorption tower [2, 3]. The two adsorption towers will be on adsorption and regeneration alternatively, to guarantee the continuous output of oxygen.

With the pressure swing adsorption gas separation technology, the gas will be separated according to the different adsorption ability of the gas on adsorbent at different pressure. It has such advantages as simple process, easy to manufacture, small floor area, quick response, simple to operate and maintain, strong adaptability, high automation, low operating cost and low investment [9].

III. MATHEMATICAL MODEL

Modelling of packed bed is the main part of any PSA process model. A simple two-bed process operated on a Skarstrom cycle is considered, as shown in the fig 1. It consists of two fixed-bed adsorbers undergoing a cyclic operation of four steps: (1) adsorption, (2) blow down, (3) purge, and (4) pressurization. By employing a sufficiently large number of beds and using more complicated procedures in changing bed pressure, PSA may be carried out as a continuous process. Hence packed bed models of various rigors have been developed first and models for any PSA process embodiment and operating conditions are developed using these packed bed models as unit modules.

Additional steps such as co-current depressurization and pressure equalization have been added to improve the purity and recovery of products as well as to make the process more energy-efficient. A common feature of all PSA processes is that they are dynamic, i.e. they have no steady state. After a sufficiently large number of cycles, each bed in the process reaches a cyclic steady state (CSS), in which the conditions in the bed at the end of a cycle are approximately the same as those at the beginning of the next cycle [7].

A. Modelling of adsorption/desorption during flow in a packed bed

The mathematical model of adsorption/desorption during flow in a packed bed of adsorbent involves mass balance equations over a differential element in the bed [3, 4]. A number of simplifying assumptions have been made for a two bed process.

1) Assumptions:

1. The system is considered to be isothermal.
2. The ideal gas law applies.
3. Frictional pressure drop through the bed is negligible.
4. Total pressure in the bed is assumed constant during adsorption and purge steps.
5. During pressurization and blow down, the total pressure in the bed varies linearly with time.
6. The fluid velocity within the bed during adsorption and desorption varies along the length of the column, as determined by the mass balance.
7. The flow pattern is represented by the axial dispersion model.
8. The equilibrium relationship for both components is represented by binary Langmuir isotherm.
9. It is assumed that argon and oxygen have the same equilibrium isotherms and therefore, the ratio of argon/oxygen remains the same as in the feed.
10. The mass transfer rate is represented by a linearized driving force (LDF) expression.

2) The basic equations [3, 5]:

The material balance for component  in the bulk phase:

\[ -D_k \frac{\partial^2 C_i}{\partial z^2} + \frac{\partial C_i}{\partial z} + \frac{\partial v}{\partial t} \frac{\partial C_i}{\partial z} + \frac{(1 - \varepsilon)}{\varepsilon} \frac{\partial q_i}{\partial t} = 0 \]  (1)

Continuity condition

\[ \sum_i c_i = C \neq f(t); \text{pressurization and blow down} \]

\[ \neq f(t); \text{adsorption and purge} \]  (2)

Overall material balance:

\[ C \frac{\partial v}{\partial t} + \frac{\partial C}{\partial t} + \frac{(1 - \varepsilon)}{\varepsilon} \sum_i \frac{\partial q_i}{\partial t} = 0 \]  (3)

Mass transfer rates:

\[ \frac{\partial q_i}{\partial t} = k_i(q_i^* - q_i) \]  (4)

Adsorption equilibrium:

\[ q_i^* = \frac{b_i C_i}{1 + \sum b_i C_i} \]  (5)

Velocity boundary conditions:

\[ v|_{z=0} = v_0, \text{Pressurization} \]

\[ = v_{0hi}, \text{High – Pressure Adsorption} \]  (6b)
\[
\frac{\partial \nu}{\partial Z} \bigg|_{Z=0} = 0, \text{ Blowdown and Purge} \quad (6c)
\]
\[
\frac{\partial \nu}{\partial Z} \bigg|_{Z=L} = 0, \text{ Adsorptoin and Pressurization} \quad (6d)
\]
\[
v|_{Z=L} = 0, \text{ Blowdown} \quad (6e)
\]
\[
v|_{Z=L} = -G \nu_{0}, \text{ Purge} \quad (6f)
\]

Boundary conditions for pressurization, adsorption and purge:
\[
D_L \frac{\partial C_i}{\partial Z} \bigg|_{Z=0} = -\nu_0 (c_i|_{Z=0^{-}} - c_i|_{Z=0^{+}});
\]
\[
\frac{\partial C_i}{\partial Z} \bigg|_{Z=L} = 0 \quad (7)
\]
\[
(c_i|_{Z=0^{-}})_{\text{purge}} = \frac{P_L}{P_H} (c_i|_{Z=L})_{\text{Adsorption}} \quad (8)
\]

Blowdown:
\[
\frac{\partial C_i}{\partial Z} \bigg|_{Z=0} = 0; \quad \frac{\partial C_i}{\partial Z} \bigg|_{Z=L} = 0 \quad (9)
\]

Initial conditions: saturated bed
\[
c_i(z, 0) = c_{i_{\text{s}}} \quad q_i(z, 0) = q_i \quad (10)
\]

**B. Solution Techniques**

The above equations are stiff partial differential equations (PDEs) with derivatives in time and space along with the boundary conditions. So, the manual solution of the above PDEs is very difficult and may not be solved by any analytical method. To overcome that problem, these stiff PDEs are converted into ordinary differential equations (ODEs).

There are several methods available to convert the PDEs into ODEs [8]. They are listed below:

1) The Finite Difference (FD) technique
2) Orthogonal Collocation (OC)
3) Orthogonal Collocation on Finite Elements (OCFE)
4) The Galerkin Finite Element (GFE) technique

All the above mentioned methods have different applications based on the type of the PDEs. This model is solved by some authors with the use of FD and OC method. The converted ODEs are being solved using different software packages. The most used packages are Visual Basic and Matlab. The result which are obtained by these methods are little different from the literature data.

**IV. A NOVEL TECHNIQUE**

As mentioned in the above section, the conversion & solution of the PDEs are difficult. To make it simpler, the all equations are converted into dimensionless quantity and then apply the OCFE technique to convert the PDEs into ODEs [7]. The conversed equations are solved using Matlab software with use of ode15s solver. The main thing is that the velocity is assumed to be constant for convenience. The equations from 1 to 10 except the equation number 6 are converted into dimensionless form after substituting the different values from equations. The dimensionless equations are listed below:

The main equations is
\[
\frac{\partial C}{\partial \tau} = \frac{1}{P_e} \frac{\partial^2 C}{\partial \xi^2} - \theta B (Q' - Q) \quad (11)
\]

The Boundary Conditions for pressurization, adsorption and purge are
\[
\text{At } \xi = 0 : C - \frac{1}{P_e} \frac{\partial C}{\partial \xi} = 0 \quad (12a)
\]
\[
\text{At } \xi = 1 : \frac{\partial C}{\partial \xi} = 0 \quad (12b)
\]

The Boundary Conditions for Blowdown is
\[
\text{At } \xi = 0 : \frac{\partial C}{\partial \xi} = 0 \quad (13a)
\]
\[
\text{At } \xi = 1 : \frac{\partial C}{\partial \xi} = 0 \quad (13b)
\]

The Initial Condition is
\[
C = 1; Q = 1 \quad (14)
\]

These set of equations are now converted into the ODEs with use of OCFE method [8]. According to the method, the bed length is divided into numbers of finite elements and each element is divided into two or three OC points. In our case, we have taken two finite elements and there are two OC points in each element. So, there are total 7 points for our range of \( \xi \) from 0 to 1. Each point has its own equations. The set of OCFE equations are listed below:

At point 2:
\[
\frac{d C_{A2}}{d \tau} = \frac{1}{P_e h_1^2} \left( 16.39 C_{A4} - 24 C_{A2} \right) + 12 C_{A3} - 4.392 C_{A4}
\]
\[
- \frac{1}{h_1} \left( -2.732 C_{A1} + 1.732 C_{A2} \right) - \theta B \left( C_{A2} - Q \right) \quad (15)
\]

At point 3:
\[
\frac{d C_{A3}}{d \tau} = \frac{1}{P_e h_1^2} \left( -4.392 C_{A1} + 12 C_{A2} \right) - 24 C_{A3} + 16.39 C_{A4}
\]
\[
- \frac{1}{h_1} \left( 0.732 C_{A1} - 1.732 C_{A2} \right) - \theta B \left( C_{A3} - Q \right) \quad (16)
\]

At point 5:
\[
\frac{d C_{A5}}{d \tau} = \frac{1}{P_e h_2^2} \left( 16.39 C_{A4} - 24 C_{A5} \right) + 12 C_{A6} - 4.392 C_{A4}
\]
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\[
\frac{1}{k_2} \left( -2.732 C_{A_4} + 1.732 C_{A_5} \right) - \frac{1}{k_2} \left( +1.732 C_{A_6} - 0.732 C_{A_7} \right) - \theta B \left( C_{A_6} - Q \right)
\]

(17)

At point 6;

\[
\frac{dC_{A_6}}{dt} = \frac{1}{P_e} \left( -4.392 C_{A_4} + 12 C_{A_5} \right) - \frac{1}{k_2} \left( 0.732 C_{A_4} - 1.732 C_{A_6} + 2.732 C_{A_7} \right) - \theta B \left( C_{A_6} - Q \right)
\]

(18)

The slope continuity condition at point 4 is,

\[
\frac{1}{k_1} \left( -C_{A_1} + 2.196 C_{A_2} - 8.196 C_{A_3} + 7 C_{A_4} \right) = \frac{1}{k_2} \left( -7C_{A_4} + 8.196 C_{A_6} - 2.196 C_{A_6} + C_{A_7} \right)
\]

(19)

Boundary conditions are,

At \( \xi = 0 \) (i.e. at point 1)

\[
\frac{1}{P_e} \left( -7C_{A_4} + 8.196 C_{A_6} - 1.96 C_{A_3} + C_{A_4} \right) = -C_{A_1}
\]

(20)

And At \( \xi = 1 \) (i.e. at point 7)

\[
\frac{1}{k_2} \left( -C_{A_6} + 2.196 C_{A_6} - 8.196 C_{A_6} + 7 C_{A_7} \right) = 0
\]

(21)

Here, we have three algebraic equations and four differential equations which we have to solve simultaneously. The manual solution may not be possible and sometimes may not be accurate. Because of this, the above equations will be solved using Matlab software.

V. FUTURE WORK

As we have discussed in the above section, the solution will be achieved by Matlab. To solve the above equations, the ode15s solver in the Matlab software will be used. The obtained result will be compared with the experimental data which was taken by doing experiments in the company named Air-n-gas process technologies at vatva, Ahmedabad.

NOMENCLATURE

- \( b_i \) Langmuir constant for component \( i \), m\(^3\)/mol
- \( B \) \( =K_a L/V \)
- \( c_i \) Concentration of component \( i \) in gas phase, mol/m\(^3\)
- \( C \) Total gas phase concentration, mol/m\(^3\)
- \( C_i \) \( = c_i/C_{i,0} \)
- \( C_{i,0} \) Initial concentration of component \( i \) in gas phase, mol/m\(^3\)
- \( D_L \) Axial dispersion coefficient, m\(^2\)/s
- \( F_{\text{exit}} \) Molar flow rate of gas at the bed exit, mol/s
- \( F_{\text{feed}} \) Molar flow rate of gas at the bed inlet, mol/s
- \( F_{\text{product}} \) Molar flow rate of product at the bed outlet, mol/s
- \( G \) Purge to feed velocity ratio
- \( L \) Bed length, m
- \( P \) (\( P_{\text{HiS}} \)) Column pressure (for high pressure step, for low pressure step), N/m\(^2\)
- \( P_e \) \( = v*L /D_L \)
- \( q_i \) Concentration of component \( i \) in solid phase, mol/m\(^3\)
- \( q_{i,s} \) Saturation limit in adsorbed phase for component \( i \), mol/m\(^3\)
- \( q_i^* \) Value of \( q_i \) in equilibrium with \( c_i \), mol/m\(^3\)
- \( Q \) \( = q_i/C_{i,0} \)
- \( t \) Time, s
- \( t_{\text{ads}} \) Adsorption duration in a cycle, s
- \( v \) Interstitial velocity in bed, m/s
- \( v_0 \) Interstitial inlet velocity during pressurization, m/s
- \( v_{OH} \) Interstitial inlet velocity during high pressure step, m/s
- \( y_{O_2} \) Instantaneous mole fraction of O\(_2\) in gas phase
- \( y_{O_2,\text{exit}} \) Instantaneous mole fraction of O\(_2\) in gas phase at the bed exit
- \( y_{O_2,\text{feed}} \) Instantaneous mole fraction of O\(_2\) in gas phase in feed
- \( z \) Axial distance from column inlet, m

Greek letters

- \( \varepsilon \) Bed voidage
- \( \xi = z/L \)
- \( \tau = t*v/L \)
- \( \theta = (1 - \varepsilon /\varepsilon_0) \)

REFERENCES


