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A Simple Equalization Pressure Prediction Method for Pressure Equalization via Tanks in PSA Process

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Abstract

Pressure equalization is one of the key steps that is being used in Pressure Swing Adsorption (PSA) processes, recently. Usage of empty tanks for pressure equalization steps is also getting more attraction due to advantages of energy saving during pressurization and to eliminate unfunctional Idle steps. Equalization pressure prediction is also very crucial for the PSA simulation. Inaccurate estimation of equalization pressure may result in deviations of gathering the real process performances. This study proposes a simple method for estimation of equalization pressure based on simple material balance on tank equalization.

Keywords: Pressure Swing Adsorption, Pressure Equalization, Tank Equalization, Equalization Pressure Prediction

1. INTRODUCTION

Pressure Swing Adsorption is a widely used reliable technology for many different gas separation purposes recently (Erden et al. 2018). Pressure equalization step in PSA cycles was first proposed back in 1966 (Berlin 1966, Stark 1966) by directly connecting two beds, one at high pressure and the other at low pressure, until their pressures equalize. A portion of the gas which would be lost in blowdown step is being used to pressurize the other bed by using less purified gas (Warmuzinski 2002, Delgado et al. 2008). Assuming the gas transferred from high pressure bed to low pressure bed is the less adsorbed (light) gas, the final equalization pressure should be the geometric mean of those two pressure values, however equalization pressure may be lower if the transferred gas is fast adsorbed (heavy). A significant saving in energy consumption can be achieved thanks to pressure equalization step, because the energy of product gas is used after the purge step instead of required mechanical energy to re-pressurize the bed at low pressure. The introduction of pressure equalization step also leads an increase in recovery of light product. Besides the advantages of introduction of pressure equalization step in the PSA cycles, equalization down and equalization up steps must match in time in the cycle schedule. However, this time alignment might put extra constraints for the cycle schedule development. The introduction of Idle steps to accommodate the pressure equalization steps results in some dead time for the gas separation process.

Empty tanks or vessels in a Pressure Swing Adsorption processes can be used not only for gas storage and recycle, but also for equalization between PSA beds. Usage of empty tank assist in aligning coupled cycle steps between bed and tanks by decreasing the number of undesirable idle steps in the cycle schedule (Ebner et al. 2018).

One of the most important prediction to be done for a PSA cycle simulation is equalization pressure estimation in the equalization steps. Adsorption simulation programs are not capable of providing accurate equalization pressures and simulating the equalization step like a conventional depressurization step. There are few studies on rough approximation of equalization pressure in equalization step, but arithmetic and geometric mean of high pressure of the bed and low pressure of the tank was also applied in literature (Bossy and Tondeur 1992, Chahbani et al. 2010, Chahbani et al. 2017, Warmuzinski, and Tanczyk 2003, Yavary et al. 2011, Yavary et al. 2015).

In this study, a model developed to have a better rough approximation of equalization pressure at the end of pressure equalization step for a PSA process including an empty tank equalization. The derived equations are based on material balance on the bed and the tank during a pressure equalization step. The results might help to understand the effect of isotherm and number of tank equalizations

2. Model

The model was developed from most basic case through the more complex systems. Hence, as a starting point; it was assumed to have only one equalization step by using an empty tank. All derivations and calculations were based on periodic steady state conditions of a cyclic PSA process.

2.1. Equalization Pressure Prediction for PSA Processes with one tank Equalization (linear isotherm)

A 3-bed 6-step PSA cycle with one equalization via tank was chosen for this theoretical study. Cycle schedule and PSA process are shown in Figure 1. PSA cycle consists of a Feed/Adsorption step in which adsorption takes place at high pressure for the heavy component. Then an Equalization down (EQd) step in which a valve between a bed and the tank opens and the bed at high pressure releases the gas through the tank until they reach the equalization pressure. The bed at medium pressure loses more gas to reach a lower pressure for gathering the heavy (strongly adsorbed) component from the adsorbed phase at the Counter-Current Depressurization (CnD) step. Light Reflux (LR) step operates for cleaning or regenerating the bed before the new cycle by purging a fraction of light product coming out from the Feed step. Then an Equalization up (EQup) step in which a valve between a bed and the tank opens and the tank at relatively higher pressure releases the gas through the bed at low pressure until they reach the equalization pressure. Finally, Light Product Pressurization (LPP) step helps to reach high pressure by using a portion of light product coming out of Feed step before starting a new cycle.

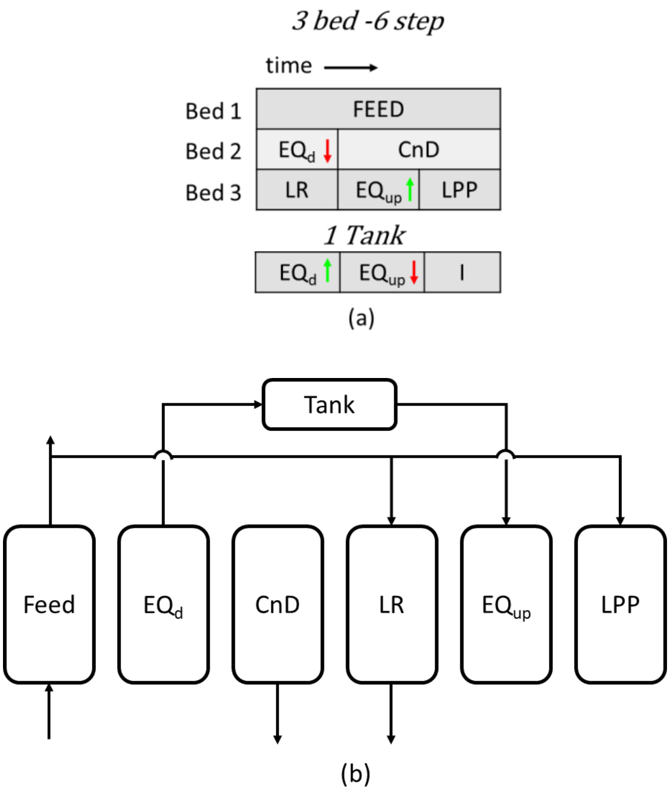

Figure 1. (a) PSA cycle schedule, (b) Schematic representation of 3 bed-6 step PSA cycle

Following assumptions have been made on Pressure Equalization step via tank before starting the material balance:

i. Number of moles leaving the bed at Equalization down step is the same as the number of moles leaving the tank at Equalization up step.

n(leaving bed) = n(supplying bed) [Equation 1]

ii. For simplicity of a model derivation, single gas (pure light component) is assumed with Linear Isotherm as seen in Figure 2.

$$q = k_h P \quad \text{[Equation 2]}$$

iii. Pressure change in the bed at Equalization up and Equalization down steps are identical because of linear isotherm and single gas assumptions.

$$\Delta P_{b1} = \Delta P_{b2} = \Delta P_b \quad \text{[Equation 3]}$$

iv. Both of pressure equalization steps were assumed as isothermal process. (T constant)
v. Ideal gas law assumption was accepted for the process.
vi. Identical beds are assumed

$$V_{b1} = V_{b2} = V_b \quad \text{[Equation 4]}$$

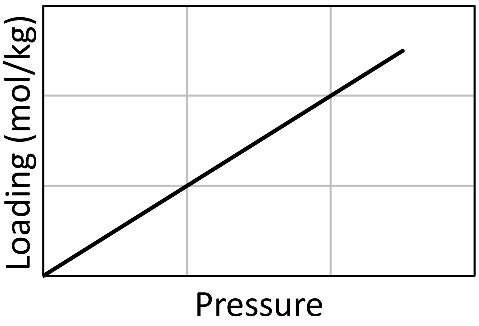

Figure 2. Single gas linear isotherm

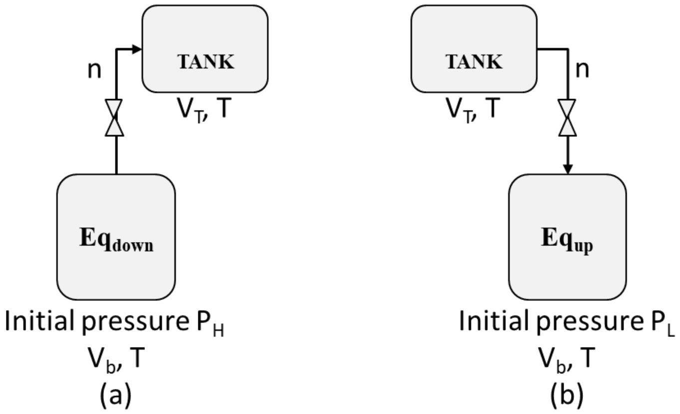

Figure 3. Schematic representation of (a) Equalization down step and (b) Equalization up step

Material balance at Equalization-down step:

$$n_T = \frac{\Delta P_T V_T}{RT} \qquad \text{[Equation 5]}$$

Where n_T is moles of gas feeding the tank from the bed at equalization down step, ΔP_T is pressure change in the tank during equalization down step, V_T is tank volume, R and T are universal gas constant and temperature, respectively.

$$n_b = \frac{\Delta P_b V_b \varepsilon}{RT} + \rho_b(1-\varepsilon)k_h V_b \Delta P_b \qquad \text{[Equation 6]}$$

Where n_b is moles of gas leaving the bed at equalization down step, ΔP_b is pressure change in the bed during equalization down step, V_b is tank volume, ε is void fraction of the bed, ρ_b is bed density, k_h is Henry's constant for linear isotherm equation, R and T are universal gas constant and temperature, respectively. The first part of the above equation reveals the gas leaving from the voids of the bed while second part of the above equation reveals the gas leaving from adsorbed phase.

Since moles of gas leaving the bed must be the same with moles of gas feeding the tank at equalization-down step, one can easily write by using Equations 5 and 6:

$$\Delta P_T V_T = \Delta P_b V_b \varepsilon + \rho_b(1-\varepsilon)k_h RT V_b \Delta P_b \qquad \text{[Equation 7]}$$

And by solving it for $\frac{V_T}{V_b}$:

$$\frac{V_T}{V_b} = \frac{\Delta P_b}{\Delta P_T}[\varepsilon + \rho_b(1-\varepsilon)k_h RT] \qquad \text{[Equation 8]}$$

On the other hand, one can easily see from the pressure history of such a PSA cycle that:

$$P_H - P_L = \Delta P_{process} = 2 * \Delta P_b + \Delta P_T \qquad \text{[Equation 9]}$$

Where P_H and P_L are highest and lowest pressure at the PSA process respectively and the difference between them corresponds to pressure change during the process ($\Delta P_{process}$).

Pressure change in the bed during an equalization step can be written as:

$$\Delta P_b = \frac{(P_H - P_L) - \Delta P_T}{2} \qquad \text{[Equation 10]}$$

For α being a coefficient between 0 and 1 to represent the pressure change in the tank divided by pressure change during the PSA process.

$$\Delta P_T = \alpha(P_H - P_L) \qquad (0 < \alpha < 1) \qquad \text{[Equation 11]}$$

$\frac{\Delta P_b}{\Delta P_T}$ term can be rearranged by substituting the Equation 11 into Equation 10:

$$\frac{\Delta P_b}{\Delta P_T} = \frac{[1-\alpha]}{2\alpha} \qquad \text{[Equation 12]}$$

Then Equation 8 turns into Equation 13 in which all other terms on the right-hand side of the equation are constants but α being variable.

$$\frac{V_T}{V_b} = \frac{[1-\alpha]}{2\alpha}[\varepsilon + \rho_b(1-\varepsilon)k_h RT] \qquad \text{[Equation 13]}$$

This equation tells that the tank volume vs. the bed volume can be easily calculated for any given PSA process parameters for a chosen α value. More importantly, equalization pressure at the end of Equalization down step ($P_{eq,down}$) from Equation 14 and equalization pressure at the end of Equalization up step ($P_{eq,up}$) from Equation 15 can be predicted if V_T and V_b are known by solving equation 13 for α value.

$$P_{eq,down} = P_H - \frac{(P_H - P_L)[1-\alpha]}{2} \quad \text{[Equation 14]}$$

$$P_{eq,up} = P_L + \frac{(P_H - P_L)[1-\alpha]}{2} \quad \text{[Equation 15]}$$

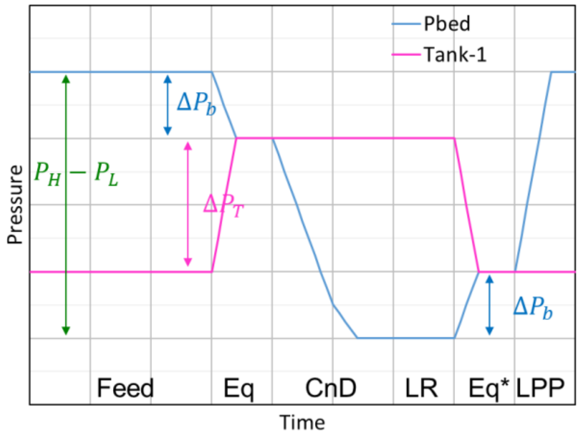

Figure 4. Pressure history representation of both a bed and the tank for one full cycle of 3-bed 6-step PSA process.

2.2. Equalization Pressure Prediction for PSA Processes with three tank Equalizations (Linear Isotherm)

A 6-bed 10-step PSA cycle with three equalizations via tanks was chosen in order to see the effect of more tank equalizations. Cycle schedule and PSA process are shown in *Figure 5*. PSA cycle consists of a Feed/Adsorption step, three Equalization down (EQ_d) steps, a Counter-Current Depressurization (CnD) step, a Light Reflux (LR) step, then three Equalization up (EQ_{up}) steps, and finally a Light Product Pressurization (LPP) step.

Same assumptions of the previous case have been assumed for deriving the model for a PSA process with more tank equalizations. Different than the previous case of with tank equalization step, pressure history (*Figure 6*) reveals that:

$$P_H - P_L = (n_{eq} + 1) * \Delta P_b + \Delta P_T \quad \text{[Equation 16]}$$

Where n_{eq} is number of equalization steps.

$$\Delta P_b = \frac{(P_H - P_L) - \Delta P_T}{(n_{eq}+1)} \quad \text{[Equation 17]}$$

$$\Delta P_T = \frac{\alpha}{n_{eq}}(P_H - P_L) \quad \text{[Equation 18]}$$

$$\Delta P_b = \frac{(P_H - P_L)\left[1 - \frac{\alpha}{n_{eq}}\right]}{(n_{eq}+1)} \quad \text{[Equation 19]}$$

$$\frac{\Delta P_b}{\Delta P_T} = \frac{[n_{eq} - \alpha]}{(n_{eq}+1)\alpha} \quad \text{[Equation 20]}$$

Hence equation 8 turns into as following:

$$\frac{V_T}{V_b} = \frac{[n_{eq}-\alpha]}{(n_{eq}+1)\alpha}[\varepsilon + \rho_b(1-\varepsilon)k_h RT] \qquad \text{[Equation 21]}$$

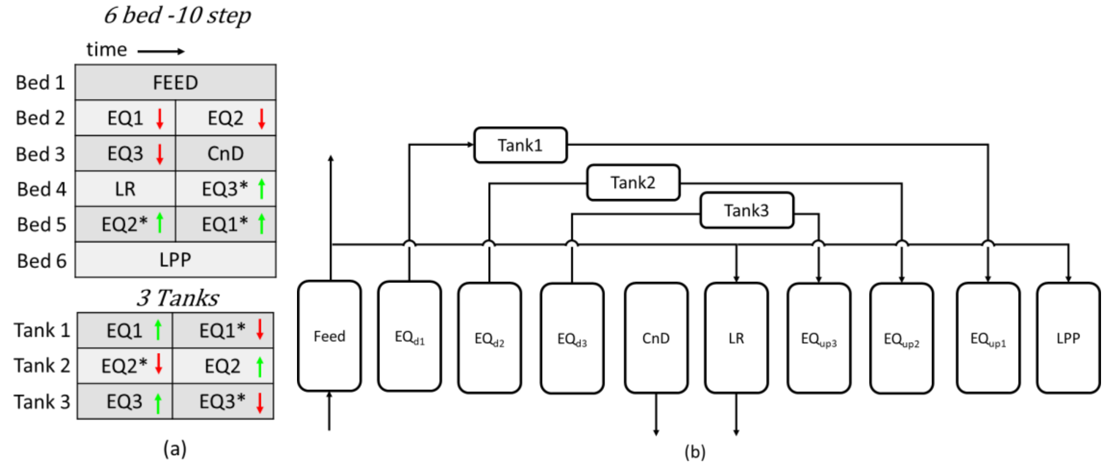

Figure 5. (a) PSA cycle schedule, (b) Schematic representation of 6 bed-10 step PSA cycle

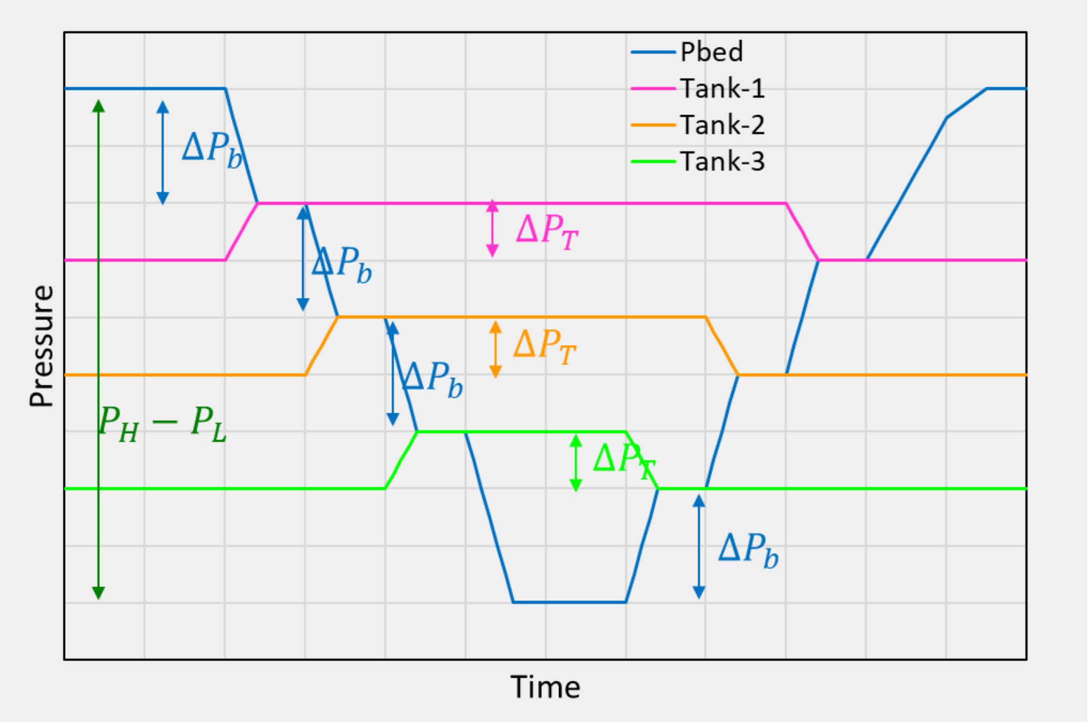

Figure 6. Pressure history representation of both a bed and three tanks for one full cycle of 6-bed 10-step PSA process.

The Equation 21 tells that tank volume vs. bed volume can be easily calculated for any given PSA process parameters and number of tank equalizations by choosing an α value. Additionally, equalization pressure at the end of each Equalization down step ($P_{eq,down}$) from Equation 22 and equalization pressure at the end of each Equalization up step ($P_{eq,up}$) from Equation 23 can be predicted if V_T and V_b are known by solving equation 21 for α value.

$$P_{eq,down1} = P_H - \frac{(P_H-P_L)\left[1-\frac{\alpha}{n_{eq}}\right]}{(n_{eq}+1)} \qquad \text{[Equation 22-a]}$$

$$P_{eq,down2} = P_H - 2\frac{(P_H - P_L)\left[1 - \frac{\alpha}{n_{eq}}\right]}{(n_{eq}+1)}$$ [Equation 22-b]

$$P_{eq,down3} = P_H - 3\frac{(P_H - P_L)\left[1 - \frac{\alpha}{n_{eq}}\right]}{(n_{eq}+1)}$$ [Equation 22-c]

$$P_{eq,up1} = P_L + \frac{(P_H - P_L)\left[1 - \frac{\alpha}{n_{eq}}\right]}{(n_{eq}+1)}$$ [Equation 23-a]

$$P_{eq,up2} = P_L + 2\frac{(P_H - P_L)\left[1 - \frac{\alpha}{n_{eq}}\right]}{(n_{eq}+1)}$$ [Equation 23-b]

$$P_{eq,up3} = P_L + 3\frac{(P_H - P_L)\left[1 - \frac{\alpha}{n_{eq}}\right]}{(n_{eq}+1)}$$ [Equation 23-c]

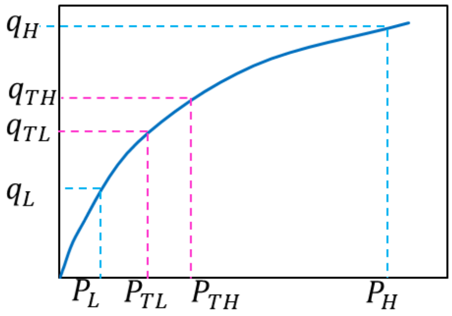

Figure 7. Single gas Langmuir isotherm (q_H, q_{TH}, q_{TL}, q_L are corresponding loadings at process high pressure [P_H], tank high pressure [P_{TH}], tank low pressure [P_{LH}], process low pressure [P_L], respectively)

2.3. Equalization Pressure Prediction for PSA Processes with Langmuir isotherm

Equilibrium based PSA processes are highly depended on the pressure changes and corresponding adsorption loading changes. A model derivation for Langmuir isotherm assumption might be more realistic. Regarding to that information following assumptions are made for the same 3-bed 6-step PSA process:

i. n(supplying tank) = n(leaving tank) which means amount of gas enters to the tank at Equalization-down step is the same as amount of gas released from the tank at Equalization-up step.

ii. Single gas (Langmuir Isotherm) assumed: $q = \frac{q_s * b * P}{1 + b * P}$ [Equation 24]

iii. $\Delta P_{b1} \neq \Delta P_{b2}$ since there is a change in pressure difference because of Langmuir type isotherm.
iv. Isothermal (T const.)
v. Ideal gas law is assumed.
vi. All beds are identical $V_{b1} = V_{b2} = V_b$

Material balance at Equalization-down step:

Amount of gas enters to the tank during Equalization-down step is: $n = \frac{\Delta P_T V_T}{RT}$

Amount of gas released from the bed during Equalization-down step is combination of both gas phase and adsorbed phase: $n = n_{gas} + n_{des}$

Hence, $n_{gas} = \frac{\Delta P_{b,down} V_b \varepsilon}{RT}$ [Equation 25] and $n_{des} = \rho_b . (1-\varepsilon) . V_b . \Delta P_{b,down} . \frac{q_s . b}{(1+bP_H)(1+bP_{TH})}$ [Equation 26]

By substituting them into Equation 1:

$$\frac{V_T}{V_b} = \frac{\Delta P_{b,down} . \varepsilon}{\Delta P_T}\left[1 + \rho_b \frac{(1-\varepsilon)}{\varepsilon} q_s bRT \frac{1}{(1+bP_H)(1+bP_{TH})}\right] \quad \text{[Equation 27]}$$

Material balance at Equalization-up step:

Amount of gas released from the tank during Equalization-up step is: $n = \frac{\Delta P_T V_T}{RT}$

Amount of gas enters to the bed during Equalization-down step is combination of both gas phase and adsorbed phase: $n = n_{gas} + n_{ads}$

Hence, $n_{gas} = \frac{\Delta P_{b,up} V_b \varepsilon}{RT}$ [Equation 28]

and $n_{ads} = \rho_b . (1-\varepsilon) . V_b . \Delta P_{b,up} . \frac{q_s . b}{(1+bP_{TL})(1+bP_L)}$ [Equation 29]

By substituting them into Equation 1:

$$\frac{V_T}{V_b} = \frac{\Delta P_{b,up} . \varepsilon}{\Delta P_T}\left[1 + \rho_b \frac{(1-\varepsilon)}{\varepsilon} q_s bRT \frac{1}{(1+bP_{TL})(1+bP_L)}\right] \quad \text{[Equation 30]}$$

By substituting Equation-30 into Equation 27 and rearranging the formula:

$$\frac{\Delta P_{b,down}}{\Delta P_{b,up}} = \frac{\left[1 + \frac{K}{(1+b(P_L+\Delta P_{b,up}))(1+bP_L)}\right]}{\left[1 + \frac{K}{(1+bP_H)(1+b(P_H-\Delta P_{b,down}))}\right]} \quad \text{[Equation 31]}$$

Where; $K = \rho_b \frac{(1-\varepsilon)}{\varepsilon} q_s bRT$ consists of only constants.

It is also known that $\Delta P_T = \alpha(P_H - P_L)$ and from pressure history representation:

$$P_H - P_L = \Delta P_{b,down} + \Delta P_{b,up} + \Delta P_T \quad \text{[Equation 32]}$$

$$\Delta P_{b,down} + \Delta P_{b,up} = (P_H - P_L)(1-\alpha) \quad \text{[Equation 33]}$$

By solving the Equation 31 and 33 simultaneously for different α values $\Delta P_{b,down}$ & $\Delta P_{b,up}$ can be found and then $\frac{V_T}{V_b}$ can be solved from Equation 30. Eventually, pressure at the end of Equalization-down step (P_{TH}) and pressure at the end of Equalization-up step (P_{TL}) can be solved by using calculated $\Delta P_{b,down}$ and $\Delta P_{b,up}$.

3. Conclusion

Accurate estimation of equalization pressure for the PSA process simulations is crucial since the inaccurate estimated values might result in deviations from actual process performances. A simple method of equalization pressure prediction at the end of equalization steps for a PSA process with tank equalization is proposed in this study. The derivation of the model was explained step by step in detail. It can be concluded that only one unknown parameter of change in bed pressure vs change in total process pressure can be evaluated if the tank size is also known. The number of equalization steps are also might be used as a parameter in the case of multiple tank equalization steps. Effect of Langmuir type adsorption isotherm was also investigated. It was seen that there is also a final equalization pressure prediction equation for the case of Langmuir type isotherm.

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