Simulation Study of Adsorption-Based VOC Removal from Industrial Painting Emissions

Dasuni De Silva, M.I. Ranathunga, A.D.U.S. Amarasinghe, and Mahinsasa Rathnayake

1 Introduction

The significance of reducing volatile organic compound (VOC) emissions has increased with the advancement of regulatory compliances and increased public understanding of their health and environmental impacts. VOCs contribute to air pollution, photochemical smog formation, and pose occupational health risks, making their control a priority in industrial operations. The paint industry, consisting of both paint manufacturing plants and painting facilities, which uses solvent-based paints is one of the major contributors for VOC emissions from manmade sources[1]

Although numerous efforts have been made to address this issue by replacing conventional solvent-based coatings with alternatives such as water-based and powder coatings, solvent-based systems remain indispensable in many industrial applications. This persistence is primarily due to their superior durability, faster drying times, and low cost[2]. Consequently, the unavoidable VOC emissions from solvent-based coating processes underscore the importance of studying potential VOC removal techniques.

Fixed bed adsorption is a proven technology utilized for VOC removal due to recoverability of adsorbent, cost effectiveness and low energy consumption. As a result, fixed bed adsorption columns are often considered as the primary solution to reduce VOC concentrations in industrial effluent gas emissions. However, these columns may become saturated or reach breakthrough concentrations in a short period under high VOC loads. Further, their performance is highly sensitive to the operating conditions such as temperature, pressure and flow rate. When the bed is unable to maintain the outlet VOC concentration below the maximum permissible limit for a considerable period, it may lead to potential frequent operational interruptions and additional operational costs. Previous studies have proposed advanced technologies to replace typical fixed bed systems such as pressure swing adsorption, temperature swing adsorption and vacuum pressure swing adsorption. However, these technologies are less feasible for small scale painting facilities due to high capital and operational costs. Therefore, assessing the performance of conventional adsorption columns for industrial painting emissions remains an important research focus. Such assessments can provide practical recommendations for optimizing breakthrough times while minimizing operational expenses.

Previous studies have identified the major VOCs emitted from industrial painting facilities [3], [4]Laboratory-scale experiments have been conducted to investigate the adsorption characteristics of both pure components and multicomponent systems. Moreover, adsorption simulations have been utilized to predict adsorption behaviour at both laboratory and industrial scales[5], [6].

However, industrial applications require a more practical perspective. In real-world air purification operations, the key objective is to ensure that the treated air remains below maximum permissible VOC limits, rather than simply maximizing adsorption capacity. Exceeding these thresholds, even if the adsorbent is not fully saturated, can lead to regulatory violations and environmental hazards. There is a lack of studies which have addressed adsorption performance with this compliance-oriented perspective under conditions representative of industrial painting operations, revealing an important gap in the current literature.

In this context, the present study focuses on simulating conventional fixed-bed adsorption systems with an emphasis on regulatory compliance. The effects of temperature, pressure, flow rate, and bed geometry on breakthrough times are analyzed to identify operational conditions that ensure VOC concentrations remain below permissible limits. This approach provides novel insights into optimizing conventional adsorption columns for real-world industrial VOC control, particularly for small- and medium-scale painting facilities where advanced adsorption technologies may be economically unfeasible.

2 Materials and Methods

2.1 Selection of VOC

As the effluent gas from painting industries contains a mixture of VOCs, most prominent species should be selected to reduce the complexity of the simulation. A two-step approach is adopted for compound selection, incorporating both industrial data and literature findings. Industrial data is acquired from a spray paint facility in Sri Lanka for four consecutive years. Some of the typical VOCs in the emissions are identified considering their abundance and presence by analyzing those data. The inlet concentrations are determined using the average data for the last four years.

The selection was verified against published data on painting facilities [3], [4]. Eight major VOCs were initially identified and categorized into four groups based on their chemical structures. A representative compound from each group was then selected according to the availability of reliable published data (see **Table 1**).

Table 1. Average concentration of VOC in emissions in the paint industry

VOCs	Representative species	Concentration (ppm)
Ethylbenzene		
Toluene	Toluene	3.93
Xylene	m-xylene	7.69
Butyl acetate		
Ethyl acetate		
1-ethoxypropan-2-yl acetate	Butyl acetate	41.15
Butanol	Butanol	7.28
Propanol		

2.2 Model Development

Aspen Adsorption software has been widely used in studies of both single- and multicomponent adsorption systems, covering a range of common adsorbents such as activated carbon and zeolites under various operating conditions at both laboratory and industrial scales. The newest version of the software, Aspen Adsorption V15 was used in this simulation.

A combination of the Ideal Adsorbed Solution Theory (IAST) and Langmuir isotherm was used to simulate the multicomponent adsorption using the single component data available in the literature. IAST accounts for competitive adsorption between species by assuming that the adsorbed phase behaves as an ideal solution, while each component follows its respective pure-component isotherm.

The IAST-Langmuir 1 model in Aspen Adsorption requires Langmuir constants; maximum adsorption capacity (q_{max}) and equilibrium constant(b) to calculate the isotherm parameters (IP1 and IP2). In Eq. (1), q represents the amount of VOC adsorbed per unit mass of adsorbent (mg/g), and P_i is the partial pressure of component i in the gas phase (Pa).

$$q = \frac{q_{max} b P_i}{1 + b P_i} \qquad \text{Eq. (3)}$$

According to previous studies, the variations of $q_{\max}$ and b are significant with temperature but negligible with pressure. [7].

One-dimensional model was used to represent the bed structure assuming convection to be the primary force for mass transfer within the bed. Linear driving force method is used to approximate the kinetic behaviour. Solid phase mass transfer coefficients(k) for the components in different temperatures are determined using,

$$\mathrm{k} = \frac{7.38 \times 10^{-8} u_o}{d_p^2} \exp\left[\Delta H \left(\frac{0.45}{RT} - 1.694 \times 10^{-4}\right)\right] \qquad \text{Eq. (2)}$$

where u_o = superficial velocity, d_p = particle diameter, ΔH = integral heat of adsorption, T = temperature and R = universal gas constant (8.314 J/kg.K)[8].

Ergun equation, valid for both laminar and turbulent conditions is used to account for the pressure drop of gas within the packed bed.

$$\frac{\partial P}{\partial z} = -\left(\frac{1.5\times10^{-3}(1-\varepsilon_i)^2}{(2r_p\varphi)^2 \varepsilon_i^3} \mu u_o + 1.75 \times 10^{-5} \mu \rho_g \frac{(1-\varepsilon_i)}{2r_p\varphi\varepsilon_i^3} u_o^2\right) \qquad \text{Eq. (3)}$$

where ε_i = porosity, μ = viscosity of gas mixture(Pa.s), ρ_g = density of gas mixture(kgm^{-3}), r_p = radius of the adsorbent particle(m) and φ = sphericity of adsorbent particle.

The software integrates Eqs. (1)–(3) along the bed length and over time to simulate the dynamic adsorption process. At each time step, it solves the mass balance for each VOC species, considering the inlet flow rate, bed geometry, adsorption capacity, and mass transfer kinetics to determine the accumulation of adsorbate within the bed. The Ergun equation is simultaneously used to account for pressure drop effects. The outlet VOC concentration is calculated directly from this mass balance, representing the fraction of VOCs that remain unadsorbed at the bed exit under the specified operating conditions of temperature, pressure, and flow rate. The breakthrough time is defined as the point at which the outlet VOC concentration reaches the maximum permissible limit.

Isothermal conditions are assumed throughout the bed during adsorption.

The adsorbent selected for this study was granular activated carbon (GAC), which has proven potential in VOC adsorption[9].

2.3 Simulations

The required input variables for the multicomponent simulation included inlet VOC concentrations (ppm), gas temperature (K), system pressure (bar), total flow rate (mol/s), adsorbent particle diameter (m), intraparticle and interparticle porosities, bed dimensions, and pure-component isotherm parameters (q_{max} and b). These parameters were user-defined prior to running the simulation.

The simulation was conducted by varying temperatures (298 – 313 K), pressures(1.5 – 3.5 bar) and inlet gas flow rates (0.1 – 1 mol/s). The breakthrough time is taken as the time at which the total outlet VOC concentration (TVOC) reached the maximum permissible limit of 5 ppm, corresponding to the emission standard applicable to Board of Investment (BOI) zones in Sri Lanka[10].

The adsorption bed is assumed to be 75 cm long with a 15 cm diameter. The particle diameter (1 mm), interparticle void fraction (0.42), intraparticle void fraction (0.20), and sphericity (1.0) are selected within the commonly reported ranges in the literature. The isotherm data (q_{max} and b) for each adsorbate related to activated carbon were determined from the literature data[5], [11].

3 Results and Discussion

Table 2. Breakthrough times for each scenario

Pressure (bar)	1.5	2	2.5	3	3.5
Breakthrough time (months)	8.7	12.9	16.6	19.3	23.3

Temperature (K)	298	303	308	313
Breakthrough time (months)	13.3	8.7	5.1	3.6

Flow rate (mol/s)	0.25	0.5	0.75	1
Breakthrough time (months)	23.7	8.7	4.1	1.9

Table 2 shows breakthrough times determined by analyzing the outlet TVOC concentration profile of the column. When one parameter is changed the other two were kept constant at, 303 K for temperature, 1.5 bar for pressure and 0.5 mol/s for flow rate.

The results indicate that the breakthrough time decreases with increasing temperature, reflecting the exothermic nature of physical adsorption[12]. In contrast, an increase in pressure prolongs the breakthrough time, as higher pressure enhances the driving force for adsorption[12]. Additionally, higher inlet gas flow rates lead to a reduction in breakthrough times. These results are consistent with trends reported in experimental studies of VOC adsorption on granular activated carbon. For example, experimental study on toluene and xylene adsorption have shown that breakthrough time decreases with increasing flow rate[5]. Further, another study conducted on benzene, xylenes and toluene depicts the same trend as the present study when the temperature and flow rate are varied[13]. Therefore, lower temperatures, higher pressures and low inlet flow rates are favourable in terms of longer lifetime of the bed.

However, maintaining these conditions is not feasible without providing the additional operational costs required to cool and pressurize air. Furthermore, the inlet flow rate is inherently limited by the operational constraints of the system. In Sri Lanka, the average ambient temperature is approximately 303 K, and operating close to atmospheric pressure (1.5 bar) is more cost-effective. Therefore, the base-case operating conditions were selected as 303 K for temperature, 1.5 bar for pressure and 0.5 mol/s for flow rate.

The optimization of bed geometry was evaluated to achieve higher breakthrough times. While maintaining the total adsorbent mass constant, varying the bed length also changes the bed diameter, resulting in different bed aspect ratios (length/diameter). This change affects the superficial gas velocity, which in turn influences mass transfer coefficients, axial dispersion, and pressure drop, leading to variations in breakthrough time (see **Table 3**). Although increasing the adsorbent mass would prolong the breakthrough time, this option is not economically viable due to the requirement of higher initial investment.

Table 3. Breakthrough time as a function of bed aspect ratio and corresponding superficial flow rate, with total adsorbent mass constant

Length of bed (m)	0.5	0.75	1	1.5	2
Aspect ratio	2.7	5	7.7	14.2	21.7

Superficial flow rate per unit area (mol/m².s)	19	28	38	57	75
Breakthrough time (months)	9.0	8.7	8.5	8.2	6.8

Since VOC concentrations in exhaust gas streams can vary with the amount and type of paint used, it is essential to assess the sensitivity of the breakthrough time to the variation of inlet concentrations. Sensitivity analysis indicates that 10% increase in inlet concentration leads to approximately 14% reduction in breakthrough time. Consequently, a significant rise in inlet VOC concentration could cause the adsorption bed to reach the breakthrough limit within a shorter period, reducing the system's practical effectiveness. This highlights the importance of avoiding conditions that lead to rapid bed saturation under elevated VOC loadings. Furthermore, it is desirable to maintain the VOC concentration of the treated gas as low as possible, even though a limit of 5 ppm was considered in this study based on regulatory requirements.

Therefore, a pre-treatment step may be required to enhance the reliability of the overall system. A practical approach is the integration of a primary adsorption stage prior to the main fixed-bed column, which can act as a preliminary filter to reduce the inlet VOC concentration before it reaches the activated carbon bed. Published literature has reported natural and low-cost adsorbents such as agricultural waste-derived biochar and modified clays with promising VOC adsorption capacities, in some cases comparable to commercial activated carbon [14], [15], [16]. Such materials could be evaluated either as a primary treatment column packaging or as a full replacement for commercial activated carbon in future studies. Therefore, future work is recommended to experimentally evaluate these alternatives and incorporate their adsorption characteristics into simulation models.

4 Conclusions

The study evaluated the feasibility of conventional fixed bed adsorption columns in removing the VOC generated in the industrial painting facilities using activated carbon as the adsorbent. Toluene, xylene, butanol, and butyl acetate were identified as representative VOCs based on industrial data and literature. IAST-Langmuir isotherm in Aspen Adsorption software was used to simulate the multicomponent adsorption behaviour of the compounds using the pure component isotherm parameters available in the literature.

The results indicate that breakthrough time increases with lower temperatures, higher pressures, and reduced inlet flow rates. However, due to economic and operational constraints, operating near ambient temperature (303 K) and moderate pressure (1.5 bar) was identified as the most practical condition. Bed geometry analysis revealed that increasing bed length at constant adsorbent mass reduces breakthrough time due to higher superficial velocity, while increasing adsorbent mass enhances performance but raises capital costs. The system performance was found to be highly sensitive to the variations in inlet VOC loading, emphasizing the need for stable inlet conditions. Incorporating a pre-treatment stage can enhance system reliability and extend adsorbent lifetime. Natural and low-cost materials such as biochar and modified clays have proven their performance in VOC removal and can be utilized as potential pre-treatment media or substitutes for commercial activated carbon. Future work should focus on experimental validation and techno-economic assessment of these alternative adsorbents.

Declaration of Competing Interest

The authors declare no competing interests.

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Credit Authorship Statement

Dasuni De Silva; Conceptualization, Data analysis, Visualization, Writing – original draft. **M.I. Ranathunga**; Conceptualization, Data analysis, Writing - editing. **A.D.U.S. Amarasinghe and Mahinsasa Rathnayake**; Supervision, Writing – review & editing.

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