

PAPER • OPEN ACCESS

A Review of mathematical models for breakthrough times of active carbon used in air conditioning

To cite this article: M Sabry *et al* 2025 *J. Phys.: Conf. Ser.* **3058** 012013

View the [article online](#) for updates and enhancements.

You may also like

- [Performance of prototype portable bio-adsorber for waste cooking oil purification](#)
R Fadhilah, E Kurniasih and M A Rifary
- [Effect of impregnated activated carbon on carbon dioxide adsorption performance for biohydrogen purification](#)
M Z Sidek, Y J Cheah, N N Zulkefli et al.
- [High-Temperature Electrochemical Studies of Metal Diffusion through Noble Metal Layers](#)
Michael Georg Stadt, Silvia Larisegger, Michael Nelhiebel et al.



UNITED THROUGH SCIENCE & TECHNOLOGY

 The Electrochemical Society
Advancing solid state & electrochemical science & technology

**248th
ECS Meeting**
Chicago, IL
October 12-16, 2025
Hilton Chicago

*Science +
Technology +
YOU!*

**Register by
September 22
to save \$\$**

REGISTER NOW

A Review of mathematical models for breakthrough times of active carbon used in air conditioning

M Sabry¹, A Elweteedy¹ and M El-ghorab¹

¹Mechanical power engineering, Military Technical College, Cairo, Egypt

Corresponding e-mail: sabrym5358@gmail.com

Abstract. Fixed-bed adsorbers which have pellets or particles with high porosity are used for adsorptive gas separation procedures. To manage and anticipate the separation results, mathematical models are used to understand the dynamics of adsorbers. The Wheeler-Jonas (WJ) equation is the most often utilized of the various models for carbon filtering that are currently known. A full set time and bed position is produced by the model as a function of flow velocity, concentration, and temperature. For this carbon material, a model is created to predict the breakthrough time, carbon bed life span, and adsorption capacity. Adsorption behavior under various operating settings was investigated by examining the reaction constant, adsorption constant, and degradation constant. The breakthrough curve for a gas with a single sorbate is obtained by solving the equilibrium isotherm and the mass and heat balance equations for the bed and sorbent particle. Each model differs from the others in terms of the kind of adsorption isotherm, whether a chemical reaction is included or excluded, whether mass transfer resistance is substantial or insignificant, the kinetics of chemical reactions, and the kind of rate law that is applied if non-equilibrium is assumed. Each model's governing equations and solution are shown and described. The tasks at hand are finding a model among the current models for carbon filtration breakthrough times and evaluating its ability to forecast penetration times of various organic and inorganic compounds. The study will demonstrate that the WJ equation can be applied to carbon filters of different sizes and applies to most chemical agents of relevance for military application.

1. Introduction

It is necessary to simulate the adsorption of the gas phase on activated carbon filters to protect all personnel, military and civilian, during military operations and/or in the case of a terrorist attack. Testing of every potential combination in a lab is simply not practicable due to the wide diversity of hazardous chemicals, ambient circumstances, and activated carbon types. The outcomes of mathematical modeling must be trusted in order to assess the level of protection offered by a particular activated carbon filter in a defined environment, accounting for the required safety margins [1].

The results of the experiment indicate that the activated carbon adsorbent's saturation adsorption capacity decreases with increasing adsorption temperature; however, the adsorption capacity of the adsorbent can still surpass 60%, and the amount of desorption may exceed 80% after continuous operation [2].

The filter is treated as a chemical reactor when describing the transport process through the filter by heat and mass transfer equations, the following set of equations can be relied upon. [2]

- ❖ A balance of mass above the filter.



- ❖ A balance of energy above the filter.
- ❖ A balance of mass above the carbon particle.
- ❖ A balance of energy above carbon particle.

This differential equation system is connected. Another equation is needed to describe the actual adsorption.[2]

Even when using modern computational methods, certain assumptions and simplifications of actual phenomena must be made, including:[3]

- A plug flow model that is unidimensional is used, meaning that there is no radial dispersion.
- The pressure drop over the filter is nonexistent. Although this is obviously untrue, pressure decrease has very little effect on the various equations.
- There is no change in the heat capacity (cp and cv). This assumption holds true within the range of the observed variations in temperature and pressure.
- There is no active contamination. This indicates that the contamination won't alter the carrier gas's macroscopic dynamic characteristics.
- The activated carbon bed and the surrounding air do not exchange heat, so the filter is regarded as adiabatic.
- At a specific location within the filter, the same temperature of both the gas and the activated carbon.

This is merely the adsorption isotherm's mathematical representation when the physisorption is pure, such as the Dubinin-Radushkevich equation. An equation describing the interaction between the carbon and the particular gas must be found in the case of chemisorption. Most of the time, a Langmuir-type isotherm can be used to fit the chemisorption equilibrium circumstances. Through the filter, a temporal concentration profile will be produced by combining these equations with the appropriate set of boundary conditions. The primary benefit of these models is that, within the bounds of the simplifications and assumptions, they simulate the entire breakthrough curve.[3]

It is necessary to understand all of the interaction parameters for the physical and chemical phenomena that occur inside the carbon. It is difficult to determine or even evaluate different diffusion coefficients, tortuosity, flow patterns, and any chemical interactions based on a limited number of studies. Because of this, only a limited number of extremely specific adsorbent-adsorbate pairings may be used with these models, which are intended to be very broad. One must start over and estimate, guess, or determine the missing parameters experimentally if either of these changes. Crucial details on the mechanisms of adsorption and transport can be obtained by carefully comparing the model's output with experimental breakthrough curves, particularly If one wants to know the values and impacts of transmission of heat and adsorption of heat via the bed [4].

Several models were used to study fixed-bed adsorption; these models were created based on different hypotheses and were only suitable in particular situations. The models that are widely used are: Thomas, Bohart-Adams, Yoon-Nelson, Wang, Zhang, and Cheng models, and the modified dose-response model[5]. The following sections describe these models:

2. Models

2.1. Wheeler – Jonas or Reaction kinetics [6]

Wheeler and Jonas's model from the early 1970s is among the most widely utilized. The Reaction Kinetic equation is another name for this equation, which has other ways of being represented. equation (1) provides the clearest one.

$$t = \frac{(W_e \cdot W)}{(Q \cdot C_{in})} - \frac{(W_e \cdot \rho b)}{(k_v \cdot C_{in})} \ln \left(\frac{C_{in} - C_{out}}{C_{out}} \right) \quad (1)$$

Where t breakthrough time (min). This equation has some restrictions [6].

- The flow pattern must have no radial diffusion and be a perfect plug flow with axial diffusion. This is typically reached when the bed's diameter is not excessively tiny in relation to its length.
- The basic concept of the original equation with physisorption into microspores.
- The rate constant k_v , must be first order in relation to the quantity of gas molecules. Typically, this holds true when c_{out}/c_{in} levels are between 5 and 10%.

Experiments can be extrapolated to different conditions, such as changing airflow, concentration, bed depth, etc. using the Wheeler-Jonas equation, we and k_v can be obtained from several ground-breaking studies and used as fitting parameters to achieve this. The required extrapolations can then be made using the values that were obtained. There must be a method to determine we and k_v without conducting any previous breakthrough experiments, though, if one is serious about forecasting breakthrough periods for a particular hazardous vapor filter system [7].

Since the static capacity, as determined by the adsorption isotherm, may be used to approximate the dynamic capacity in the case of physisorption, this problem is not too difficult for We to answer. Consequently, we can be computed using the Dubinin-Radushkevich equation in a fairly simple manner equation (2):

$$We = W_o dL \exp\left[-\frac{BT}{\beta^2} \log^2\left(\frac{C_s}{C_{in}}\right)\right] \quad (2)$$

w_o and B are the only parameters that are uncertain, dL and C_s are tabulated. These can be obtained from any known activated carbon isotherm. The affinity coefficient β can be computed or obtained in the literature. It is more challenging to estimate the total mass transfer coefficient k_v . Differentiating between the several diffusion phases in the adsorption process is impossible from the outset. Thus, semi-empirical formulae are used to estimate k_v . The most comprehensive one to date is provided by equation (3).

Where M_w is the molar mass of the toxic organic vapor (g.mol^{-1}) of the Dubinin-Radushkevich equation and d_p is the mean diameter of the carbon particles (cm) [8].

$$K_v = 800 B^{0.33} d_p^{-1.5} V_L^{0.75} \left(\frac{M_e}{M_w}\right)^{0.5} \quad (3)$$

Neither theoretical nor experimental diffusion models can be used to correlate k_v . Stated otherwise, the model is not physically accurate. However, it is particularly helpful to explicitly distinguish between kinetics and capacity when researching new systems and/or how specific parameters affect the adsorption behavior [1]. Since we are only looking at one filter and one compound at a time at a fixed flow rate, the filter parameters are kept constant. Thus, the WJ equation can be expressed as follows:

$$t_b = A - B \ln\left[\frac{C_{in} - C_{out}}{C_{out}}\right] \quad (4)$$

Accordingly, we may use curve fitting or linear regression to fit equation (4) to the data in order to estimate coefficients A and B . The constants we and k_v may now be determined from the fitted equation at low outlet concentrations using [9]:

$$A = \frac{W \cdot W_e}{Q C_{in}} \quad \rightarrow \quad We = \frac{Q A C_{in}}{W} \quad (5)$$

and

$$B = \frac{W_e \rho_b}{K_v C_{in}} \rightarrow K_v = \frac{W_e \rho_b}{B C_{in}} \quad (6)$$

2.2. Zhang model [10]

The elimination of cyanogen chloride from a gas stream that passes over a bed of activated carbon impregnated with copper, chromium, and silver is described by this model, which will be investigated in this study in the context of hydrogen sulfide adsorption [10].

The model is predicated on the idea that the absorption process proceeds in two separate ways: a first-order catalytic deactivation reaction of the poisonous gas and the physical adsorption of cyanogen chloride by activated carbon. The deactivation rate equation is:

$$\frac{\partial \phi}{\partial t} = K_d \phi \quad (7)$$

Where Φ is the deactivation function (dimensionless)

With the initial condition set to $t = 0$, $\Phi = 1$, and the integration of (equation 7) yields (equation 8) for the deactivation function. The following solution holds true for separable deactivation kinetics caused by contact with a catalyst poison at a constant concentration (inlet concentration) with no spatial variation.

$$\phi = e^{-K_d t} \quad (8)$$

The chemical reaction follows a first-order reaction and the rate equation is:

$$R = KC\phi = KCe^{-K_d t} \quad (9)$$

Where K is the reaction rate constant (s^{-1}). Assuming that the bed dynamics are isothermal and that there is no axial dispersion, the surface gas velocity remains constant, and the fixed bed adsorber's continuity equation is as follows:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + \frac{1-\varepsilon}{\varepsilon} \rho \frac{\partial q}{\partial t} + R = 0 \quad (10)$$

Where ε is bed porosity (dimensionless), q is the adsorbate concentration in the carbon (g adsorbate/g carbon), and ρ is the bulk density of the carbon (g/dm³). Since the Langmuir isotherm is linear at low concentrations, the physical adsorption is defined by a linear isotherm.

$$q = K_i C \quad (11)$$

Then taking the derivative of equation (11) versus time, the following expression is,

$$\frac{\partial q}{\partial t} = K_i \frac{\partial C}{\partial t} \quad (12)$$

Where K_i is the adsorption constant in (L gas/g carbon). The above partial differential equation (10) was solved by Zhang [10]. Using the streamline method and the boundary conditions below.

- At $x = 0$, $t > 0$, $C = C_0$
- At $t = 0$, $x > 0$, $C = 0$

The following solution is given below

$$\ln \ln \frac{C_0}{C} = \ln \frac{K}{\left[1 + \frac{K_i \rho (1-\varepsilon)}{\varepsilon}\right] K_d} - K_d t + \ln \left\{ e^{\frac{K_d x \left[1 + \frac{K_i \rho (1-\varepsilon)}{\varepsilon}\right]}{u}} - 1 \right\} \quad (13)$$

The breakthrough curve is linearized and expressed as follows if bed height x remains constant:

$$\ln \ln \frac{C_0}{C} = a - K_d t \quad (14)$$

Where

$$a = \ln \frac{K}{\alpha K_d} + \ln \left(e^{\frac{K_d \alpha L}{u}} - 1 \right) \quad (15)$$

$$\alpha = 1 + \frac{K_d \rho (1 - \varepsilon)}{\varepsilon} \quad (16)$$

Where L is the length of the bed (dm)

2.3 Adam and Bohart Model [11]

A popular model for describing adsorption kinetics during chemical reactions was developed by Adam and Bohart for one-component adsorption. It was discovered that the first portion of the breakthrough curve for numerous one-component adsorption systems including chemical reactions may be described by this model. Any solute adsorbed onto the carbon surface cannot desorb, according to the irreversible adsorption isotherm included in the model. Though many are sharp enough to support modeling systems with irreversible assumptions, no real isotherm in the world is totally irreversible [11]. The equation below is for mass balance for the fixed bed adsorption column.

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} + \frac{1 - \varepsilon}{\varepsilon} \frac{\partial q}{\partial t} \quad (17)$$

Kinetics of adsorption is described using the quasichemical rate law below:

$$\frac{\partial q}{\partial t} = KC(q_e - q) \quad (18)$$

Where q_e is the constant value of q (g adsorbent/L carbon), and k is a constant. According to the quasichemical rate law, the adsorbate concentration in the gas and the percentage of the adsorbent's capacity that is still present at any given time determine the rate of adsorption. The model uses the rectangular irreversible isotherm normally used to describe the reaction system.

$$q_e = \{0, c=0\}, \{q_s, c>0\}$$

The differential mass balance solved for negligible axial dispersion

$$\frac{C}{C_0} = \frac{\exp(\tau)}{\exp(\tau) + \exp(z) + 1} \quad (19)$$

Where

$$\tau = k C_0 \left(t - \frac{x}{u} \right) \quad (20)$$

And

$$z = \frac{k q_s x}{u \left(\frac{1 - \varepsilon}{\varepsilon} \right)} \quad (21)$$

By re-arranging the above equation (19) the linear form below is obtained.

$$\ln \left(\frac{C_0 - C}{C} \right) = -kC_0 \left(t - \frac{x}{u} \right) + \ln \left\{ \exp \left[\frac{kq_s x \varepsilon}{u(1-\varepsilon)} \right] + 1 \right\} \quad (22)$$

By plotting $\ln (C_0 - C/C)$ versus $(t - x/u)$, a linear relationship is expected if the Adam and Bohart model fits the experimental data.

2.4 Thomas Model [12]

Thomas developed a model that uses Langmuir isotherm for equilibrium and ion exchange-based second-order reversible reaction kinetics. The continuity equation of the column is written as,

$$v \frac{\partial c}{\partial x} + \frac{\partial c}{\partial t} + \frac{\rho}{\varepsilon} \frac{\partial q}{\partial t} = 0 \quad (23)$$

The adsorption kinetics is described as,

$$\frac{\partial q}{\partial t} = k_1 (q_0 - q)c - k_2 q(c_0 - c) \quad (24)$$

Where k_1 and k_2 are velocity constants (s^{-1}), c_0 is the inlet concentration of adsorbate in the gas stream (g adsorbate/L) and q_0 is the initial ion exchange capacity of the carbon (g adsorbate/g carbon). Both favorable and unfavorable adsorption circumstances can be used with the given expression, which depicts second-order reversible reaction kinetics and assumes a constant separation factor. Adsorption is often governed by interphase mass transfer rather than the kinetics of chemical reactions. As a result, Thomas' model works well for adsorption processes without internal or external diffusion constraints [12]. The initial boundary conditions for the system are stated below.

- At $t = 0$, $x \geq 0$, $q = 0$
- At $x = 0$, $t \geq 0$, $c = c_0$

Thomas solved the above continuity problem by assuming plug flow and negligible axial dispersion, yielding the following answer for long bed lengths,

$$\frac{C}{C_0} = \frac{1}{1 + \exp[k_T(q_0 m_c - C_0 V_{eff})/Q]} \quad (25)$$

Where k_T is the Thomas rate constant ($dm^3 / (s \cdot g)$), m_c is the mass of carbon (g), q_0 is the adsorptive capacity of the carbon (g/g), V_{eff} is the throughput volume (L). The above equation can be linearized to give,

$$\ln \left(\frac{C_0}{C} - 1 \right) = \frac{k_T q_0 m_c}{Q} - k_T C_0 t \quad (26)$$

Where $V_{eff}/Q = t$. A plot of $\ln (C_0/C - 1)$ vs. t of the experimental data, should, assuming the above model is accurate, provide a linear relationship.

2.5 Yoon and Nelson Model [13]

Yoon and Nelson's theoretical model is predicated on gas adsorption kinetics and the idea that the rate at which the probabilities of adsorption for each molecule decreases is related to the probability of the sorbate adsorption and sorbate breakthrough on the sorbent [13]. It follows that,

$$-\frac{dQ}{dt} \propto QP \quad (27)$$

Where Q (%) is the probability for adsorption, t (s) is time, and P (%) is the probability of breakthrough. Experimental data indicates that the rate at which the likelihood of adsorption decreases is inversely related to the weight of the carbon W_c (g adsorbent) and directly proportional to the gas contaminant concentration C (g adsorbate/L) and the volumetric flow rate U (L/s) [13]. Therefore,

$$-\frac{dQ}{dt} \propto \frac{CU}{w_c} QP \quad (28)$$

By introducing a dimensionless constant of proportionality k , we have

$$-\frac{dQ}{dt} = \frac{kCU}{w_c} QP \quad (29)$$

Or

$$-\frac{dQ}{dt} = k_{YN} QP \quad (30)$$

Where

$$k_{YN} = \frac{CU}{w_c} \quad (31)$$

Using the boundary condition to solve the above differential where at 50% breakthrough, $t = t_{0.5}$, $Q = Q_{0.5}$, and $P = P_{0.5}$. The following solution is obtained, Where C_0 is the inlet concentration (g adsorbate/L gas).

$$\ln \left(\frac{C}{C_0 - C} \right) = k_{YN} t - t_{0.5} k_{YN} \quad (32)$$

3. Breakthrough curve

The breakthrough curve is the mirror image of the adsorption front. It expresses concentration at the filter outlet as a function of time[1]. The majority of military applications and general protective applications do not require simulation of the entire breakthrough curve. When the breakthrough curve reaches a particular concentration, known as the breakthrough concentration, which is the point of interest. This is a fixed value that varies depending on the hazardous chemical. It seems sense that this is the level of concentration at which the wearer of the protective gear begins to feel negative effects.

3.1. Factors to Consider When Choosing the Correct Theoretical Model

Choosing the suitable theoretical model for the process studied depends on the assumption of equilibrium or non-equilibrium behavior, the type of rate law for non-equilibrium, the type of adsorption isotherm, and the existence of axial dispersion or not.

The right model for the process being studied can be established by examining the experimental breakthrough curve, determining its shape, and employing trial and error. Kinetic parameters that take into consideration axial dispersion, internal and exterior mass-transfer resistances, and the impact of adsorbate deposition on catalyst degradation can be determined by the use of experimental breakthrough curves. These constants are necessary for the model to be fully solved, which enables usage in process design, scale-up, and simulation studies. A comprehensive collection of flow velocity and concentration data are produced as a function of time and bed location is produced by the model [14].

When equilibrium theory is applied, there is instant equilibrium between the bulk flow and the adsorbed phase, and the bed becomes in an equilibrium state. For quick adsorption processes unhindered by mass transfer resistances, this assumption holds true. The solution and adsorbent phases across the bed are assumed to be in equilibrium to solve fixed-bed adsorption issues. This criterion is met if the adsorbate is quickly absorbed or if the solution has a lengthy residence time in the bed, meaning no resistance. If the equilibrium is maintained, one has $q = f(c_b)$.

3.2 Problems with Breakthrough Modeling.

3.2.1 Humidity.

The impact of humidity on breakthrough times is significant. A concentration of roughly 16550 ppm of water molecules is equal to a relative humidity of 62% at 297 K, which is not at all inflated and is actually very typical in most regions of the world. Through the inhaled air stream, this concentration interacts with the activated carbon in a filter. The activated carbon in clothes and filters will therefore be exposed to water vapor even in the absence of any harmful substance. This is frequently referred to as the carbon bed's pre-wetting or pre-humidification. In the event of a chemical accident, the poisonous component will compete with the pre-adsorbed water and the water vapor in the air stream. It is possible to simulate the decrease of adsorption capability in the case of physisorption. Volume exclusion is the most effective method for accomplishing this [15].

Every effect of water on the adsorption kinetics will be converted into a decline in k_v values. The water adsorbed on the carbon will also affect adsorption kinetics by slowing down mass transfer [16].

3.2.2 Discontinuous flow pattern.

Because of a change in the overall mass transfer coefficient k_v , experimentally determined breakthrough times with a "breather" flow (discontinuous or half-sine flow) have occasionally been demonstrated to be noticeably shorter than the breakthrough time with corresponding flow [4].

3.2.3. Chemisorption, Chemical reaction, and trace quantities.

A mass balance throughout the carbon bed is the foundation of the Wheeler-Jonas equation. It should therefore still be applicable in the case of chemisorption; nevertheless, a priori, neither the equation nor the K_v equation can be applied in this situation. The K_v equation and we equation appear to be true in certain situations, most notably when the rate-controlling phase in the chemisorption process is diffusion rather than the chemical reaction [17].

3.3 Parameters affecting the adsorption/desorption process.

3.3.1 Influence of Adsorption Temperature on Adsorption Effect.

Generally speaking, the operating temperature has an impact on the adsorption capacity. To obtain adsorption isotherms, volatile organic compounds were adsorbed by activated carbon at regulated temperatures [18]. According to Figure 1, within a specific range, the adsorption temperature can have a significant effect on the adsorbent's penetration time. The adsorption penetration time of activated carbon reduces as the temperature rises. The adsorbent's adsorption capacity decreases by 18.5% as its adsorption process temperature rises by 10 °C. The adsorption capacity of the adsorbent is significantly influenced by the adsorption temperature. To increase the adsorption capacity of the adsorbent, the adsorption temperature in the industrial adsorption process should be lowered as much as feasible [2].

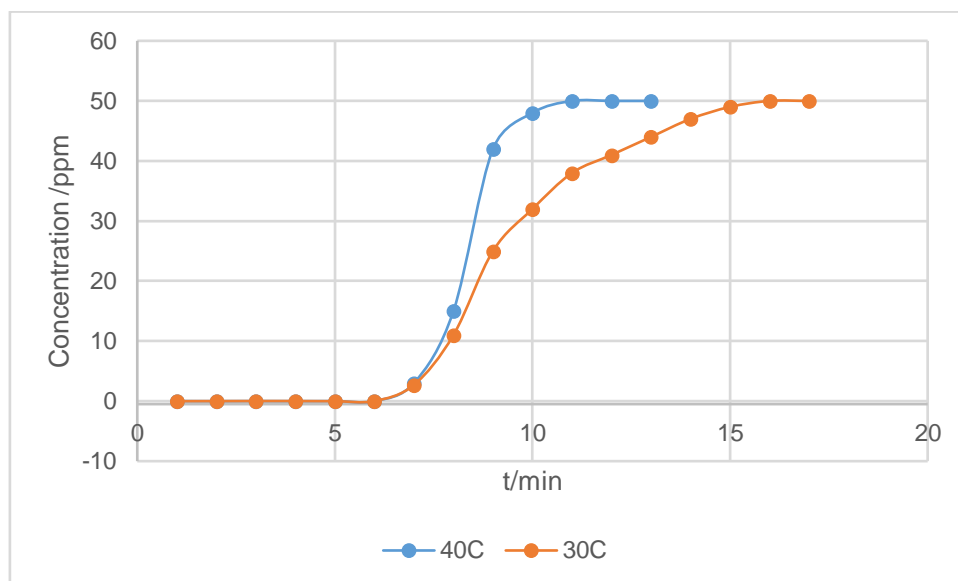


Figure 1. Breakthrough curves of active carbon at different adsorption temperatures [2]

3.3.2 Desorption Temperature's Effect on the Desorption Effect.

Figure 2 shows that when the desorption temperature rises during the operation, the maximum value of the outflow concentration rises as well. The highest value of the desorption concentration is 3711 ppm at a desorption temperature of 100 °C, and 850 ppm and 2100 ppm at desorption temperatures of 70 °C and 90 °C, respectively [19]. The quantity of desorbed steadily diminishes as the desorption temperature drops under various conditions. The desorption duration increases primarily because the desorption temperature gradually drops, molecular thermal movement decreases, and the attraction between molecules and activated carbon increases. Activated carbon desorption curves at various temperatures [2].

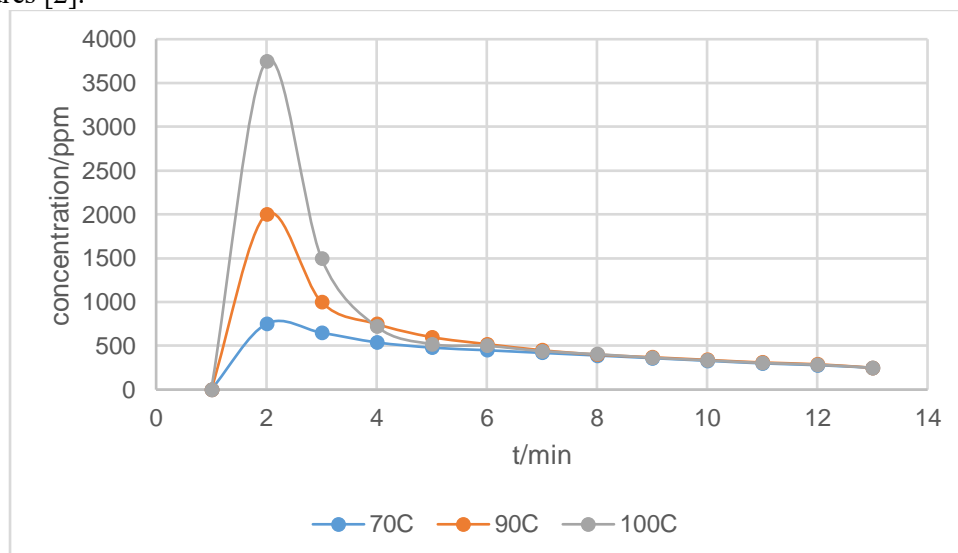


Figure 2. Breakthrough curves of active carbon at different desorption temperatures[2]

3.3.3 Impact of Adsorption/Desorption Durations on the Treatment Outcome of VOCs.

The activated carbon exhibits good adsorption/desorption cycle performance since, after ten cycles of adsorption and desorption, the adsorbent's adsorption capacity can exceed 60% and its desorption

capacity may come over 80% (apart from the initial desorption). Additionally, the first time is the activated carbon's maximum first adsorption capacity [2].

4. Conclusion

Each model has the condition that makes it give the best results, for example (WJ) model gives good results when output concentration is low, but Zhang assumes bed dynamics are isothermal and that there is no axial dispersion using the first-order deactivation function. For Adam's model, assume irreversible adsorption isotherm with chemical reaction. Thomas' model works well for adsorption processes without internal or external diffusion constraints, assuming plug flow it uses Langmuir isotherm for equilibrium and ion exchange-based second-order reversible reaction kinetics. Yoon's model used experimental data and theoretical models to relate the probability of sorbate adsorption and sorbate breakthrough on the sorbent. Slowing down mass transfer, the water deposited on the carbon has an effect on adsorption kinetics. And decreasing adsorption capacity. Also, the discontinuous flow has shown that it makes breakthrough time shorter. The adsorption temperature affects on penetration time and adsorption capacity, both of them decrease when temperature increases. For desorption, the quantity of desorbed decreases as the desorption temperature drops under various conditions.

References

- [1] H Adsorbents 2005 *Combined and Hybrid Adsorbents*. Kiev, Ukraine: springer
- [2] M J K B Editors 2023 *Environmental Pollution Governance and Ecological Remediation Technology*. doi: 10.1007/978-3-031-25284-6.
- [3] D Kaplan, I Nir and L Shmueli 2006 Effects of high relative humidity on the dynamic adsorption of dimethyl methylphosphonate (DMMP) on activated carbon vol. 44, pp. 3247–3254, doi: 10.1016/j.carbon.2006.06.036.
- [4] Y Suzin, I Nir and D Kaplan 2000 The effect of flow pattern on adsorption of dimethyl methyl phosphonate in activated carbon beds and canisters vol. 38, pp. 1129–1133.
- [5] K Erme, R Hanke-, K Sundmacher, J St-pierre and B Wetton 2017 Mathematical modelling and simulation on the adsorption of Hydrogen Sulfide (H_2S) gas Mathematical modelling and simulation on the adsorption of Hydrogen Sulfide (H_2S) gas doi: 10.1088/1757-899X/206/1/012069.
- [6] P Lodewyckx, G O Wood and S K Ryu 2004 The Wheeler – Jonas equation : a versatile tool for the prediction of carbon bed breakthrough times vol. 42, pp. 1351–1355, doi: 10.1016/j.carbon.2004.01.016.
- [7] F Stampfer, I Hygiene, S Group and L Alamos 1993 ADSORPTION RATE COEFFICIENTS FOR GASES AND VAPORS ON ACTIVATED CARBONS vol. 31, no. I, pp. 195–200.
- [8] P Lodewyckx and L Verhoeven 2003 Using the modified Wheeler–Jonas equation to describe the adsorption of inorganic molecules: chlorine vol. 41, pp. 1215–1219.
- [9] L Leopold 2017 Analysis of respiratory filters by the Wheeler-Jonas equation Department of Physics.
- [10] H Zhang and D Cheng 2000 Mathematical model for a fixed bed adsorptive reactor vol. 38, pp. 877–880.
- [11] A Of and T H E Be 1920 SOME ASPECTS OF THE BE RESPECT TO ~~~ O.
- [12] S Bashkova, T R Armstrong and V Schwartz 2009 Selective Catalytic Oxidation of Hydrogen Sulfide on Activated Carbons Impregnated with Sodium Hydroxide no. 22, pp. 1999–2007, .
- [13] Y H E E. Yoon and J H Nelson 2010 Application of Gas Adsorption Kinetics I . A Theoretical Model for Respirator Cartridge Service Life vol. 8894, doi: 10.1080/15298668491400197.
- [14] I Sorbents 1987 CHAPTER 2 Adsorbents and Adsorption Isotherms doi: 10.1016/B978-0-409-90004-0.50005-2.
- [15] B Poszwald, A Kwak, K Dysz and A Dylong 2023 Effect of Impregnation of Activated Carbon with Selected Transition Metal Ions on Its Adsorption Properties and Pore Size *Mater.*

- Res. Proc.*, vol. 34, pp. 87–94, doi: 10.21741/9781644902691-11.
- [16] X Song, D Liu, G Zhang, M Frigon, X Meng and K Li 2013 Bioresource Technology Adsorption mechanisms and the effect of oxytetracycline on activated sludge *Bioresour. Technol.*, vol. 151, pp. 428–431, 2014, doi: 10.1016/j.biortech.10.055.
- [17] P Zhang 2022 The Adsorption of VOCs by Honeycomb Ceramics Loaded vol. 2022.
- [18] S Huang, T Chung and H Wu 2021 Effects of Molecular Properties on Adsorption of Six-Carbon VOCs by Activated Carbon in a Fixed Adsorber doi: 10.1021/acsomega.0c06260.
- [19] Y Li, H Jin, W Liu, H Su, Y Lu and J Li October 2017 Study on regeneration of waste powder activated carbon through pyrolysis and its adsorption capacity of phosphorus pp. 1–7, 2018, doi: 10.1038/s41598-017-19131-x.

Nomenclature

B	Pore structure of adsorbent	u	superficial velocity (dm.s ⁻¹)
C _{in}	Inlet concentration (g _{gas} .cm ⁻³)	V	Linear rate of flow of gas (m/s)
C _{out}	Breakthrough concentration (g _{gas} .cm ⁻³)	v	Superficial velocity of the gas (cm.s ⁻¹)
C ₀	Inlet concentration (g _{dsorbate} /L)	V _{eff}	Throughput volume (L)
c	Adsorbate concentration in the gas (g _{gas} .cm ⁻³)	We	Adsorption capacity (g _{gas} /g _{carbon})
d _p	Mean diameter of the carbon particles (cm)	W	Total mass of carbon in the filter (g)
K _v	Overall mass transfer coefficient (min ⁻¹)	W _o	Micro pore volume of adsorbent (L)
K _d	Deactivation rate constant (s ⁻¹)	x	Distance from the bed inlet (dm)
K	Reaction rate constant (s ⁻¹)	Q	Probability for adsorption
K _i	Adsorption constant (L _{gas} /g _{carbon})	P	Probability for breakthrough
k ₁ , k ₂	Velocity constants (s ⁻¹)	d _L	Liquid density
M _w	Molar mass of the toxic organic vapor (g.mol ⁻¹)		
m _c	Mass of carbon in the column (g)	q _e	Constant value of q
v _L	Linear velocity of the air stream through the bed (cm.s ⁻¹)		
Q	Volumetric flow rate (cm ³ . min ⁻¹)	c _s	Saturation concentration (g _{gas} .cm ⁻³)
q	Adsorbate concentration (g _{adsorbent} /L _{carbon})		
R	Reaction rate (g/Ls)		

Greek letters

ε	Bed porosity	β	Affinity coefficient
ρ _b	Bulk density of the carbon (g _{carbon} .cm ⁻³)		