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Estimating the Service Life of Activated Carbon Filters for Air Purification

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Abstract

It is very important to be able to predict the breakthrough time of gas mask filters under real life circumstances. This article describes the use of a very simple predictive equation, the Wheeler-Jonas equation, that yields excellent predictions but only within a very restrictive set of boundary conditions. In order to make this model work in a more realistic environment, it has been gradually adapted to take into account a number of parameters related to this environment: a non-constant inlet concentration, a breather flow, new physical forms of activated carbon, the relative humidity and temperature of the ambient air, chemisorbed gases and mixtures of organic vapours. As (nearly) all of these parameters can be calculated independently of each other, based on data that are either readily available or that can be measured, their influence on the complexity of the model stays low. This makes this combined model both easy to use and powerful in predicting breakthrough times of gas mask filters under real-life conditions.

1. Introduction

When dealing with toxic compounds in the air, it is considered best practice to avoid this health risk altogether. However, in practice, this is not always feasible. This is the case in industry where workers cannot always avoid entering a toxic environment. But this usually happens under well-defined and known circumstances, i.e. the protective equipment, particularly the filter associated to the gas mask and the profile of its use, can be tailored toward the risk. This is a lot less straightforward when the situation is not controlled, e.g. in case of an accidental industrial release or when soldiers (and civilians) are faced with an attack with chemical weapons. The latter can happen during military operations or can be the result of a terrorist action.

In these cases, it is of the utmost importance to estimate the time that people are protected, i.e. how long they can stay in a certain area once the accident or the attack has occurred. A lot of attention and research has been dedicated to modelling the behaviour of toxic clouds, based on the source of the toxic cloud, the nature of the toxic and meteorological and geographical data. Models exist on both the source term – how the cloud is formed – and the subsequent movement and changes in concentration. This has led to good estimates of concentration-time-spatial coordinates profiles (i.e. what the concentration of the toxic will be at a certain place, at a certain time). These profiles can be, in turn, used as entry variables in mathematical models predicting the behaviour of protective equipment; in particular, gas mask filters filled with activated carbon.

Nowadays, the rapid evolution of computers and their calculation capabilities have made it possible to develop very accurate models for the behaviour of gasses inside a filter. This behaviour is typically described by a set of mutually interlinked (partial) differential equations that deal with the transfers of mass and energy inside the filter. Solving this set of equations is usually done by some type of finite elements approximation. However, although computation strength becomes less and less an issue, these models are still rarely used to predict the real-life behaviour of filters. The main problem is that they require some parameters (e.g. tortuosity,

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or a good knowledge of adsorption heats) that are rather difficult to obtain. When the exact circumstances are known, a limited number of experiments can suffice to determine them. But usually these circumstances are not known on beforehand or rather, there is a near infinite number of possible circumstances possible in the real-life use of filters. Therefore, other models have been developed. The latter are less sophisticated, usually leading to less good and correct estimations of the behaviour of the gas inside the filter. But this downside is largely compensated by the fact that they need far less input parameters and that these parameters are rather easy to determine.

Usually, these models are what one can call "integral" models. I.e. they are not going to calculate the exact concentration, adsorbed amount and temperature in each point of the filter, but consider it a black box that is described by a number of parameters. Parameters that can be estimated, ideally on a purely theoretical basis. If this is not possible, one should be able to do this with a minimal number of experiments.

In practice, the protection offered by a filter against a toxic compound is expressed by a single value, known as the breakthrough time. This is the time between the moment the toxic contacts the inlet of the filter and the moment that the concentration of the toxic at the outlet of the filter (i.e. in the air that will be inhaled by the person wearing the gas mask) reaches a predetermined value. This value is usually linked to the concentration of the toxic that will pose an immediate or long-term health risk.

2. The model

The general model that was chosen is the so-called Wheeler-Jonas model [1]. This model has been around for many years (dating from the 1970's) but is still one of the best and most robust ones. This is because it requires a limited number of parameters, especially of the ones related to the adsorbent (see further).

The Wheeler-Jonas equation is given as Eq. 1. The physical meaning of this equation is illustrated in Fig. 1. This figure depicts the concentration at the outlet of the filter as a function of time. If adsorption kinetics would be infinitely fast ($k_v = \infty$), the breakthrough time would be t_2, the time equal to the first term of Eq. 1. This would be the case of a perfect plug flow. In reality, there is axial diffusion and when the bed is becoming saturated, the front will be proceeded by a mass transfer zone. As usually the toxicity level of the gases and vapours lies well below the concentration in the air (otherwise a gas mask would be unnecessary), the breakthrough time t_b will be shorter than t_2, usually near t_1, the moment the first gas molecules will penetrate the filter.

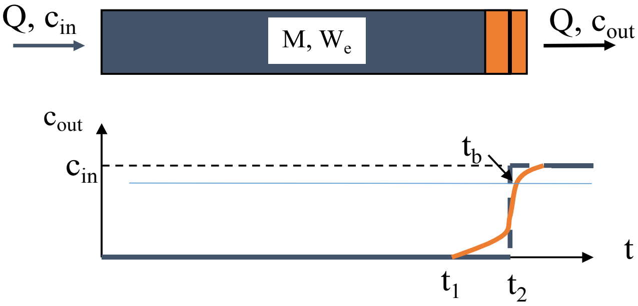


Fig. 1. Graphical representation of the breakthrough time of a gas through a filter and its elation with the parameters of the Wheeler-Jonas equation.

This model does not take into account the radial dispersion (i.e. according to the model the breakthrough will occur simultaneously over the whole outlet surface of the filter. It has been shown that this is not completely correct [2], but is the case of commercial filters (i.e. with grain sizes smaller than 1/50 of the filter diameter) radial dispersion can be neglected:

$$t_b = \frac{W_e.M}{Q.C_{in}} - \frac{\rho_b W_e}{k_v.C_{in}}.ln\left(\frac{C_{in} - C_{out}}{C_{out}}\right) \qquad (1)$$

Here t_b is the breakthrough time to reach C_{out} (min), M the weight of the carbon bed (g_{carbon}), W_e the equilibrium adsorption capacity of the carbon for the given vapour (g/g_{carbon}), Q the volumetric flow rate (cm^3/min), C_{in} the concentration of the vapour in the air (g/cm^3), C_{out} the chosen breakthrough concentration (g/cm^3), ρ_b the bulk density of the carbon bed (g_{carbon}/cm^3) and k_v the overall adsorption rate coefficient (min^{-1}). Normally all parameters for a specific application are either known (M, Q, ρ_b), can be measured (C_{in}) or are chosen (C_{out}), except for the capacity W_e and the pseudo-first order kinetic constant k_v. The former is in fact the point on the organic vapour adsorption isotherm for this specific adsorbent, corresponding to the measured (or known) inlet concentration C_{in}. This point can be accurately estimated from the isotherm of any other purely physically adsorbed vapour based on the Polanyi or Volume Filling of

Micropores theory [3]. As such, Eq. 2 – the Dubinin-Radushkevich equation, can be used to calculate W_e if the relevant parameters of the micropore distribution (W_o and B) have been determined, e.g. by measuring a N_2-isotherm at 77 K [4].

$$W_e = W_o.d_L.exp\left[\frac{-BT^2}{\beta^2}.log^2\left(\frac{C_s}{C_{in}}\right)\right] \qquad (2)$$

With W_o the measured micropore volume (cm^3/g_{carbon}), d_L the liquid density of the organic vapour (g/cm^3), B the measured structural constant of the carbon (K^{-2}), T the temperature (K), β the affinity coefficient of the organic vapour (-) and C_S the concentration of the contaminant corresponding to the saturation vapour pressure of the contaminant P_S (g/cm^3). The other parameters are those from Eq. 1. The parameter β, a measure for the attraction between the carbon and the adsorbate, is tabulated or can be estimated from the molar polarization method [5].

The latter parameter, the pseudo-first order kinetic constant k_v, is more difficult to estimate. Various semi-empirical models have been developed, based on different rate controlling steps in the adsorption mechanism [6, 7]. Several years ago a new equation (Eq. 3) was developed, based on inter- and intraparticle diffusion. This equation gives the best fit for a very large array of experimental data [8].

$$k_v = 800.\beta^{0.33}.v_L^{0.75}.d_p^{-1.5}\left(\frac{W_e}{M_w}\right)^{0.5} \qquad (3)$$

With v_L (cm/s) the linear velocity of the air flow through the carbon bed, d_p (cm) the mean diameter of the carbon granules, M_w (g/mole) the molecular weight of the organic vapour and the other parameters those of Eqs. 1 and 2.

If, for some reason, it is impossible to determine the different parameters, especially W_e and k_v, theoretically or by means of measuring a nitrogen isotherm they can be determined experimentally. Breakthrough times under different conditions can be used to calculate W_e and k_v by using Eqs. 1 to 3 in a reverse way. But this should constitute a last resort as clearly one loses much of the advantage of having predictive equations, avoiding unnecessary testing.

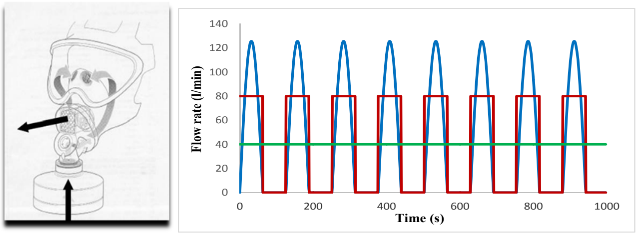
Although it is clear from literature [9] that this simple equation is quite powerful in predicting breakthrough times for a wide range of toxic compounds, under different conditions, it presents some major drawbacks. Most of them are related to limitations on its applicability.

The first one is the inlet concentration C_{in}. Contrary to what is expected in Eq. 1, this value of the inlet concentration will not be constant, as usually the toxic compound will be passing as a cloud, or the person wearing the gas mask will enter this cloud. In both cases, concentration will rise gradually from zero to a maximum plateau value followed, in the best case, by an equally gradual drop.

The second one is the flow rate Q. Flow rate (and the ensuing v_L) are considered to be constant too. In reality, the flow through a filter is not constant, but presents itself as a half-sine breather flow (exhaling occurs through an exhaust valve in the mask, at zero flow through the filter), see Fig. 2. Here the horizontal line corresponds to a constant flow. On a side note, one can question the common practice of testing filters (e.g. for quality assurance purposes) with such a constant flow. Indeed, the real flow through the filter will be dictated by the opening and closing of the exhaust valve. The combination of this valve being open or shut (which are, of course, not absolute but present some transition phenomena during opening and closing) and the natural sinusoidal breathing rate will lead to a flow through the filter that is situated somewhere between the half-sine and the block flow depicted in Fig. 2 [10].

A third one is the physical form of the activated carbon. Up to a few years ago, all activated carbon used in air filtration was in a granular form as this was judged to be the optimum solution for both fast adsorption kinetics and (reasonably) low breathing resistance. Over the years, new forms have been developed, with either faster kinetics (e.g. fibres) or lower breathing resistance (e.g. carbon monoliths), the notion of particle diameter d_p (see Eq. 3) becoming void.

Other important influences, not accounted for in the equation, are the relative humidity of the air stream and the temperature. The latter is present in the first term (as part of the isotherm equation) but seems strangely enough absent in the kinetic part of the equation.



(a) (b)

Fig. 2. The real flow through a gas mask (a) and the resulting flow pattern (b).

Finally, the equation is only valid for a single, physically adsorbed, vapour. As many toxic compounds, especially in an industrial environment, are non-organic gases, they are not (or hardly) adsorbed on pristine activated carbon. Instead, these gases require chemical interactions with specific impregnations on the carbon (e.g. metal complexes) in order to be retained. Mixtures of vapours and/or gases also constitute a problem, as the different compounds will compete for adsorption space in the available micropore volume and/or for chemical interactions with the impregnants.

3. Experimental work

Over the last 25 years, several hundreds of breakthrough measurements were performed by our research group alone. International collaboration [11, 12] has led to a database of several thousands of breakthrough data. This is important as all models are of the semi-empirical kind. We define this as models that are based on a theoretical analysis to determine which parameters, influencing the adsorption behaviour (i.e. present in the Wheeler-Jonas equation), could be sensitive to the initial parameter (e.g. temperature, humidity, co-adsorbed vapour,…) under investigation. In a second stage, these parameters are varied during a predetermined set of experiments in order to derive the exact nature of the dependence of the breakthrough time on the initial parameter, via the Wheeler-Jonas parameters. Finally, the model and its parameters are verified by a second set of experiments, varying other parameters of the Wheeler-Jonas equation, to make sure that no parameters were overlooked and the established model is generally applicable.

4. Results and discussion

We will look at the different weaknesses of the Wheeler-Jonas model one by one, trying to find ways to estimate breakthrough times even though the original model not being valid under these circumstances.

4.1. Non constant inlet concentration

Breakthrough tests were performed with concentrations increasing step-wise between 0 and 5000 ppm with steps of 500 or 1000 ppm and variable step lengths (see Fig. 3).

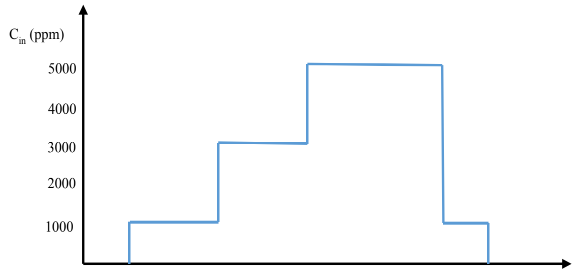


Fig. 3. One of the concentration profiles used in the experiments to determine the influence of a non-constant inlet concentration of the toxic compound.

The model (Eqs. 1–3) was applied with the mean value of the inlet concentration between t = 0 and t = t_b. In all cases, experimental and modelled breakthrough times were in very close agreement. When using the model to predict breakthrough times, this introduces a supplementary problem, as one needs the breakthrough time in order to calculate the mean value of the inlet concentration between the donning of the mask and the breakthrough time. This means the model will need a loop on the linked values of t_b and $\overline{c_{1n}}$, but this does not constitute a major problem, as in all tested cases this loop quickly (2–3 iterations) reached a solution and no cases of instability were detected [13].

4.2. Non constant flow rate

There has been a lot of discussion on the influence of the breather flow. Some research groups did not find any significant differences between the experimental breakthrough times with a (real) breather flow and a constant flow, whereas others did find substantial differences [14,15]. In most cases, filters are not tested with a real half-sine flow, but rather with a pulse (or block) flow (see Fig. 2). An extensive literature search, combined with many breakthrough tests with both pulsed and continuous flows, has shown the rationale behind the differences: the adsorption kinetics. The latter will influence the width of the mass transfer zone. However, when the mass transfer zone is small compared to the overall depth of the filter (i.e. big filters), this difference in mass transfer zone will hardly be noticed in the breakthrough time. If, on the other hand, the filter is shallow, the width of the mass transfer zone (i.e. the second term of Eq. 1) will become more important, and there will be a marked effect on the breakthrough time.

This is illustrated in Fig. 4 where the ratio between the breakthrough times for a pulsed and continues flow is plotted against the carbon weight, i.e. the depth of the filter, for a specific set of testing

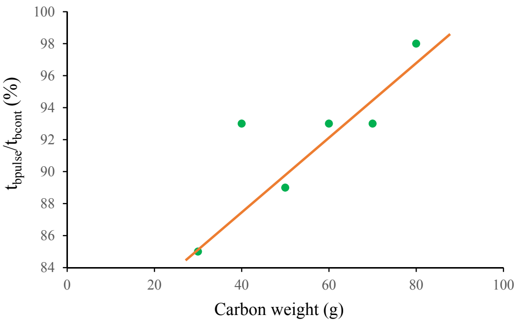


Fig. 4. Influence of filter depth on the ratio of the breakthrough time under pulsed and continuous flow conditions.

conditions. The result at 40 g can be discarded as an outlier. It is clear that, under these conditions, when the amount of carbon reaches 80 g the difference between the two types of flow essentially disappears (t_{bpulse} and t_{bcont} are roughly equal taking into account the measurement uncertainty). For 30 g, this difference is situated around 85%, i.e. a 15% faster breakthrough in the case of a pulsed flow.

An examination of the different equations (1 through 3) reveals that only the parameter v_L is directly related to the flow pattern and will influence k_v, and thus t_b. Theoretically one can determine the mathematical difference between the average of $(v_L)^{0.75}$ between t = 0 and t = t_b and $(v_{Laverage})^{0.75}$ for a half sine flow or a block flow they amount at 18% for the former and 15% for the latter. From Eqs. 1 and 3 it is clear that this difference will be translated in a difference of the same magnitude for the breakthrough time if the second term of Eq. 1 is approximately equal to the first one. Which is the case of the experiments shown in Fig. 4. So one can notice the excellent agreement between the theoretical and experimental values of $t_{bpulse}/t_{bcontinuous}$.

Based on this result, one can use a correction factor of 1.22 (= 1/0.82) when estimating the real breakthrough of a filter used in combination with a gas mask, i.e. using $(1.22\ v_L)^{0.75}$ instead of $(v_L)^{0.75}$ in Eq. 3 [16].

4.3. Non granular activated carbons

Examining the different equations, it is clear that the only parameter being influenced by the physical form of the carbon is the particle diameter d_p in Eq. 3. Looking at the theoretical background of this equation, d_p is related to the diffusion rate of the contaminant from the bulk of the gas phase to the surface of the particle. As such, it is a measure of the contact surface.

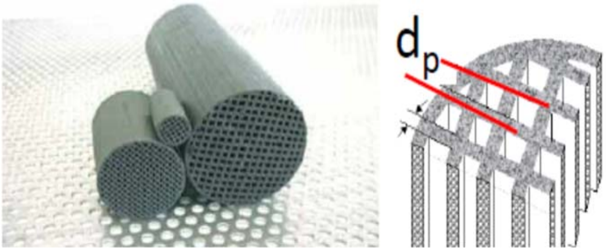


Fig. 5. The value of d_p in the case of carbon monoliths.

In the case of non-spherical particles (e.g. extrudates) one has to use an equivalent diameter: this is the diameter of a spherical particle with the same external surface.

For a carbon monolith, d_p should be replaced with the inner diameter of the channels (see Fig. 5), whereas for carbon fibres the determining parameter would be the (average) length of the fibres, their diameter having a negligible contribution to the external surface. These assumptions have been proven experimentally for non-spherical particles [17], activated carbon monoliths (ACM) [18] and activated carbon fibres (ACF) [13].

4.4. Air stream humidity

The relative humidity of the airstream, and any influence of previously adsorbed water, are absent from Eqs. 1 to 3, because they were established for the adsorption of one single vapour from a matrix of non- (or very weakly) adsorbed gases. In general, air (N_2, O_2,…) does respond to this criterion. Adding the fact that the carbon surface is known to be very hydrophobic, one could imagine limited interference by ambient water vapour. However, the combination of the fact that the carbon surface is never free of heteroatoms (acting as initiators for water adsorption) and that water vapour is usually abundantly present in the ambient air, leads to a filling of the micropore system of the activated carbon by adsorbed water during the normal use of a gas mask [19, 20]. For volatile toxic organic compounds this can lead to a drop in breakthrough time of more than 90%, i.e. the filter losing nearly completely its ability to protect against this vapour. This is illustrated in Fig. 6 for the breakthrough time of CCl_4 on a non-impregnated activated carbon (Calgon BPL) for different levels of pre-humidification (0 – 20 – 50 – 70 – 80 and 90% Relative Humidity): the initial (dry) breakthrough time of around 200 min drops to approximately 7 min in the worst case scenario of a pre-humidification at 90% RH and a contaminated air stream at 90% RH. This pre-humidification mimics the fact that a filter has been in use before being challenged by a toxic vapour. This is normally not the case in an industrial environment where gas masks are usually donned just before entering the toxic environment. But in military applications, troops can await a chemical attack for several hours. During this time, the usually high concentrations of water vapour in the ambient air pass through the filter and can interact with the activated carbon. As water vapour adsorption on activated carbon is a slow process, the influence of this pre-humidification is more important than the interaction during the actual filter use, i.e. the co-adsorption with the toxic compound.

This effect has been modelled. The basis of this model being an exclusion-substitution equilibrium. In short, the part of the micropore volume that is filled with water is unavailable to the vapour. This means that the amount of adsorbed water has to be subtracted from the parameter W_o in Eq. 2 (= exclusion). Unless the vapour is more strongly adsorbed than water. In this case it will be able to replace the water, totally or partially (= substitution). The degree of replacement depends on the ratios of C_{in} and P_s (or C_s) as can be deduced from Eq. 2. Higher concentrations of a less volatile compound will chase off some of the (pre-)adsorbed water, whereas inverse conditions of the toxic chemical will make it less prone to make this substitution. Again (see 4.1), the calculation of breakthrough time will require a loop. Whereas the pre-adsorbed water can be calculated independently (as it was adsorbed before t = 0 = start of the presence of the toxic compound), this is not the case for the amount of water adsorbed between t = 0 and t = t_b. To calculate this amount, both t_b and the kinetics of water adsorption have to be determined. As explained earlier, the first one will require a loop (on t_b and the amount of water adsorbed), and the latter needs a good insight in the process of water adsorption on activated carbon, including the establishment of semi-empirical equations for the water vapour adsorption kinetics [21].

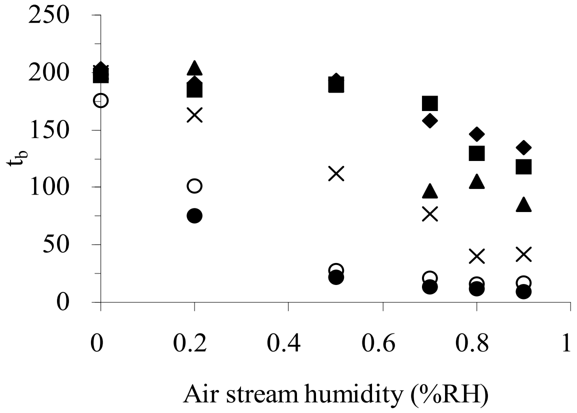


Fig. 6. Breakthrough time of CCl_4 as a function of the pre-humidification (0▲-20■-50▲-70x-80○-90●%) of the carbon and the humidity of the air stream.

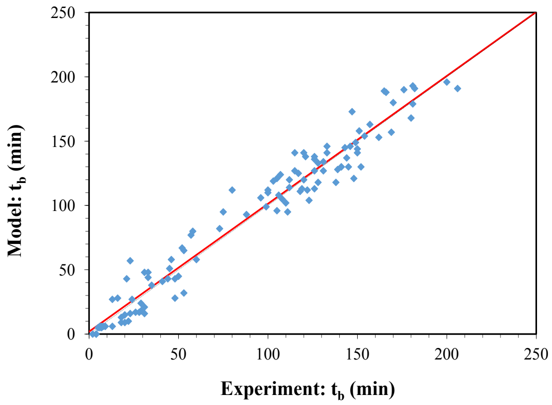


Fig. 7. Comparison between experimental and modelled breakthrough times in the presence of water vapour.

To complicate things, the adsorption kinetics of the toxic vapour (Eq. 3) will also be influenced by the water vapour present inside the pore system of the activated carbon. Notwithstanding the various problems (e.g. the loop on t_b) the resulting model [22, 23] stays relatively simple and requires a limited number of experimentally determined parameters to yield very accurate predictions of the real breakthrough time in the presence of ambient humidity. This is illustrated in Fig. 7 where more than 100 experimentally determined breakthrough times (under humid conditions) are compared to the results of the model.

4.5. Temperature

As for the impact of temperature, this seems to be rather straightforward as Eq. 1 is directly influenced by Eq. 2. This is quite logical, adsorption being an exothermal process, higher ambient temperatures will lead to lower amounts of the toxic compound being adsorbed. Hence, this part of the influence of temperature is already present in the initial Wheeler-Jonas equation.

But it seems strange that Eq. 3, representing adsorption kinetics, is apparently independent of temperature. Moreover, none of the parameters (except for W_e, but that is accounted for through Eq. 2) can be expressed as a function of temperature. Hence, only the pre-exponential term (800) could be influenced. Preliminary research in this area has started recently, and the first results seem to indicate that this term presents a negative correlation with temperature, i.e. kinetics become slower with increasing temperatures. This is, of course, totally counterintuitive. One possibility is an underestimation of the influence of W_e in Eq. 3 (the difference between zero filling and a filling of the micropore system equal to W_e being the driving force for the adsorption), but further research is necessary to elucidate this apparent inconsistency. However, the model, although presenting some weird features, seems to work quite well on several data sets. So it seems that the temperature dependency can be mathematically modelled by adapting Eq. 3, making it possible to accurately predict breakthrough times under different temperatures.

4.6. Non physically adsorbed gases

Finally, one has to tackle the problem of the equations being only valid for one single, physically adsorbed, vapour. In fact, there have been attempts to use the Wheeler-Jonas equation for non-physically adsorbed gases [24]. As one can see, Eq. 1 is in fact very general, i.e. it can be used for any type of gas adsorption, provided W_e and k_v are known. Which implies that, even if they are not known, Eq. 1 can still be used to extrapolate experimental data, providing one sticks to changing the other parameters of Eq. 1, leaving all non-directly represented parameters (e.g. T, RH,…) untouched. But estimations of breakthrough times can be made if W_e and k_v are either measured or calculated. The latter still seems to be impossible at this moment, as the exact nature of the interactions between the gas, the carbon, carbon surface complexes and other features (such as impregnated metal salts) is in most cases unknown, and certainly not quantifiable. But the value of W_e is known if one has measured an isotherm of this gas on that particular carbon, even if it has no link anymore with Eq. 2. Generally speaking, it is neigh impossible to measure such isotherms for all gases on all types of activated carbon. But it is indeed possible to obtain these data for a selected number of gases (e.g. with high toxicity and/or very common use in industry) on the limited amount of carbons that are most commonly used in gas mask filters. Measuring k_v is less straightforward as it usually requires a lot of experiments, unless it has been shown experimentally that the physical adsorption of the gas is the rate controlling step of the total adsorption process. In this case, Eq. 3 can indeed be used to calculate k_v. If not under all circumstances, than certainly under the normal circumstances (e.g. c_{in}) of the use of the filter [25].

Some attempts have been made to quantify the influence of the adsorption of a chemically adsorbed substance on the physisorption of a second compound, and vice versa, but this has only led to some qualitative conclusions. The general trend being that, whatever type of adsorption and compounds involved, there will be, at best, no influence, at worst a severe shortening of the breakthrough time of either, or both, compounds. The "best case scenario" being a purely chemisorbed gas and a purely physisorbed vapour. But usually there will be an influence. The main reason for this mutual influence is the fact that chemisorption is always preceded by some form of physisorption as the gas has to be retained in place long enough for the reaction to take place (similarly to gas-gas reactions in the presence of a catalyst). In some cases, the impregnation acts as a catalyst, e.g. by hydrolysing molecules such as NH_3. The corresponding products being less volatile, they can be physically adsorbed and are thus retained by the filter. Again, it is clear that there will be a competition for available micropore space between these reaction products and a co-adsorbed organic vapour. On top of that, two gases moving simultaneously through the micropore system of the carbon will clearly affect each other's kinetics. This leads always to a (although small) reduction of both breakthrough times, even in the aforementioned "best case scenario".

4.7. Mixtures of physisorbed vapours

Things are clearer when dealing with a mixture of two (or more) physisorbed vapours. Here an adapted version of the exclusion-substitution model that was used in the case of the co-adsorption with water vapour could be applied. Indeed, the replacement of the weaker adsorbed vapour by the more strongly adsorbed has been reported in literature since many years as it is obvious from the two breakthrough curves (see Fig. 8).

The weaker adsorbed does not only break through at an earlier time (due to the loss of micropore volume occupied by the more strongly adsorbed one), but whatever was adsorbed is (partially) replaced. This results in the so-called roll-up phenomenon [25].

More recently, this phenomenon has also been demonstrated inside a filter [26]. This is illustrated in Fig. 9.

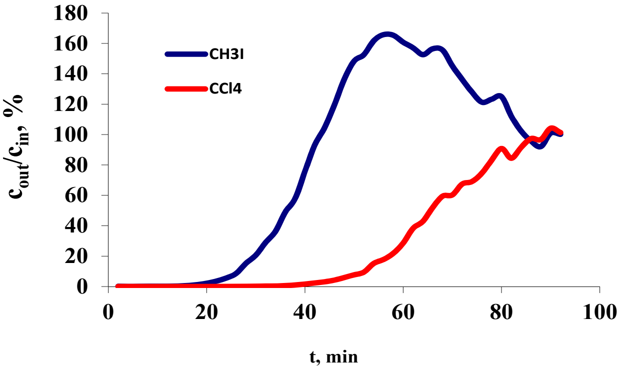
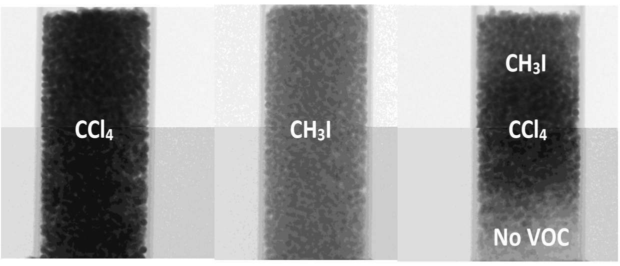


Fig. 8. Co-adsorption of 2 organic vapours, resulting in a roll-up phenomenon of the more weakly adsorbed vapour.

As such, co-physisorption has been studied both qualitatively and quantitatively. Some of the former results are shown in Fig. 10. They show essentially two things. First of all that both vapours each follow the general trends predicted by a Wheeler-Jonas equation. And, equally important, that the only parameters influencing the co-adsorption behaviour are the relative concentrations of the two vapours and their affinity towards the activated carbon (i.e. how well they are adsorbed).These are essentially the same two parameters that have been used in the exclusion-replacement model of the water-vapour co-adsorption.

Therefore, the model that was used to take the ambient humidity into account has been adapted to describe this, and gives very good results when the affinities of the vapours for adsorption on activated carbon differ significantly, i.e. when their saturation vapour pressures are very dissimilar. When they are very close, complex substitution phenomena come into play, influencing both W_e and k_v. These are still under investigation but, overall, the mathematical expressions that have been found seem to allow for reasonably accurate prediction of the breakthrough time of both vapours [27].



(a) (b) (c)

Fig. 9. (a) – CCl_4 adsorption; (b) – CH_3I adsorption; (c) – co-adsorption of CCl_4 and CH_3I with roll-up of CH_3I.

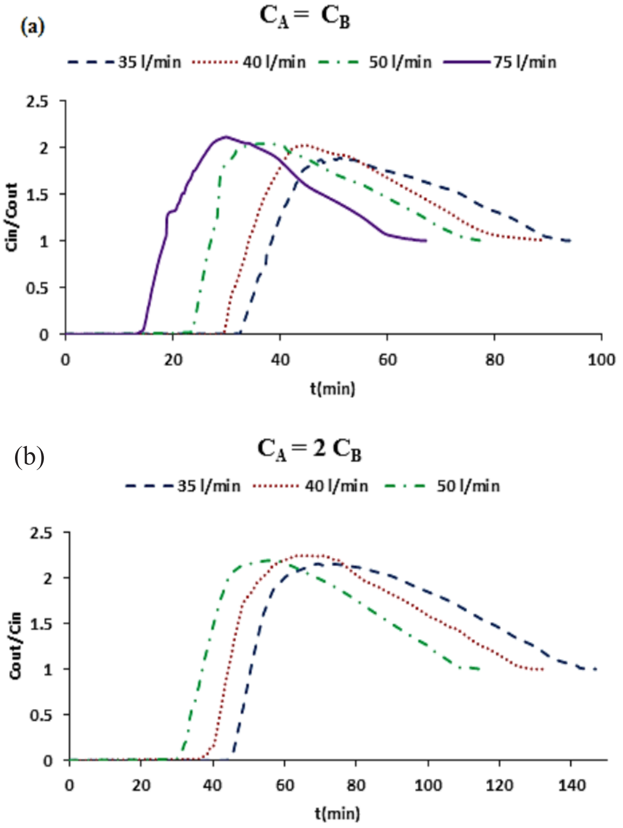


Fig. 10. Qualitative interpretation of binary co-adsorption of organic vapours (A = $C_2H_4Cl_2$; B = C_7H_{16}) showing the influence of the flow rate for (a) equal and (b) different inlet concentrations of the vapours.

Clearly, in order to describe what happens in real life circumstances, both models (vapour-vapour and water-vapour co-adsorption) should be combined as the vapour-vapour co-adsorption will nearly always take place in ambient air, i.e. air containing a reasonable to high amount of water vapour.

5. Conclusions

The Wheeler-Jonas equation is a very simple predictive equation that yields excellent predictions but only within a very restrictive set of boundary conditions. To make this model work in a more realistic environment, it has been gradually adapted and improved to take into account a number of parameters related to this environment. Some problems still need solving (e.g. chemisorption) or fine-tuning (e.g. influence of temperature, co-adsorption), but most boundary conditions (non-constant inlet concentration, breather flow, new physical forms of activated carbon, relative humidity) have been integrated in the model. As (nearly) all of the aforementioned parameters can be calculated independently of each other, based on data that are either readily available in literature or that can be measured, their influence on the complexity of the model stays low. In fact, a simple Excel-sheet suffices to calculate the estimated breakthrough time in all cases presented in this article. This makes this final model both easy to use and powerful in predicting breakthrough times of gas mask filters under real-life conditions.

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