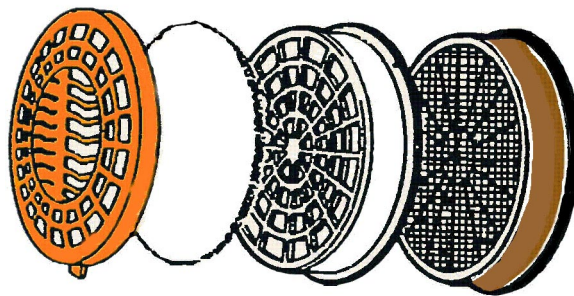




The Practical Use of some Existing Models for Estimating Service Life of Gas Filters

Calculations of
Adsorption Capacity and
Breakthrough Times



September 1997
Safety Equipment Australia Pty Ltd

Abstract

A lot of work has been done regarding estimating service life of gas filters. Almost all of this work is about organic solvents. There have also been a lot of tests made to verify the calculation models. There is a lot of useful information to collect for the users of gas filters but is it really utilized?

At SEA we have made an overview regarding estimation of service life for gas filters. Some of the information we found was used to make a model for estimating service life using a PC spreadsheet (Microsoft Excel). The spreadsheet contains existing, well-known models for calculating adsorption capacity and breakthrough times for single substances. It also contains a possibility to compensate the adsorption capacity and breakthrough time for humidity in the air. This model has been an excellent tool in many cases, both in practical workplace issues and when informing people about the function of gas filters.

Introduction

How long will the filter last? This is the first question that comes up when someone is mentioning the word gas filter. The normal way to detect a breakthrough in the filter is to rely on the warning properties of the substance the filter shall protect against. This means that when the user senses taste, smell or irritation in the mouth or nose there is a breakthrough and the filter should be changed. The problem with this is that there are big individual differences in how sensitive people are. There are also a lot of substances that do not have any warning properties at all, or only at to high level.

An alternative method is to calculate the service life of the filter. Is this possible with sufficient accuracy? The answer to that question is **Yes, but.....**

There are also a lot of other situations when one wants to estimate the service life of the gas filters. What filter life can I expect if I use a class 1 filter instead of a class 2 filter? What filter life can I expect if I change the concentration of the solvent? What can I expect to happen if I change from solvent X to solvent Y?

We have made an overview of the methods available to calculate service life for gas filters, and put some of them together in a Microsoft Excel workbook. This workbook is an excellent help in understanding more about how gas filters work, and it also fully illustrates the difficulties in calculating the gas filter life times in real workplace situations.

Most of the scientific work in this field concerns the adsorption of organic solvents in pure activated carbon and a number of different calculating methods for this case can be found in the literature. Therefore the greatest part of this work will be about organic solvents. Finally, anyone familiar with breakthrough time calculations understands the complex nature of this matter. For this reason we must warn against using these figures alone for deciding when filter a change shall be made. You must **never override or ignore** the warning properties of the substance you are using the filter against.

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Estimation of adsorption capacity by calculation with the D/R equation

The first step when calculating breakthrough times for gas filters is to establish the **adsorption capacity**. The abbreviation for this is W_e and it represents the amount of solvent the carbon contains when it is saturated (in equilibrium) with a certain concentration of the solvent. The unit for W_e is grams solvent / grams carbon.

The best value for W_e is from a test using the same concentration and for the same type of carbon for which we are calculating breakthrough times. Another way is to pick a value from literature or from other tests as similar as possible to the case we are calculating.

If no reliable values can be found one can make a calculation based on the structure of the activated carbon and the properties of the solvent. The following input data is required for such a calculation (with the equation we are using).

$$W_e = \rho W_o \exp \left\{ - \frac{BT^2}{\beta^2} \left[\log \left(\frac{p_s}{p} \right) \right]^2 \right\}$$

Equation 1. The Adsorption capacity

- **Affinity coefficient (β).** Test results can be found for some solvents but often it must be calculated. This is done automatically in the spreadsheet but you must manually enter the calculated value in the cell "Affinity coefficient". If you have a test result or table value you want to use, enter that instead. The calculation is done by correlating to the properties of benzene. This is a

standard method for calculating the affinity coefficient.

- **Saturated vapour pressure (p_s).** This can be found in chemical handbooks and databases.
- **Density of solvent (ρ).** Same as above.
- **Molecular weight of solvent (M).** Same as above.
- **Solvent vapour pressure (p).** This is calculated automatically when you enter the challenge concentration.
- **Maximum adsorption space (W_o).** This value tells how much adsorption space the carbon has and it can be obtained from the carbon suppliers or from literature for similar carbon types. The value is normally in the range 0.4 to 0.75 and a typical value is around 0.6 cm³/g.
- **Degree of porosity (B).** This is a porosity constant for the carbon and it can be obtained from the carbon suppliers or from literature for similar carbon types. This value is correlated to the "Maximum adsorption space" and when that is 0.6 this value normally is around 1 to 1.2 E-06.
- **Temperature (T).** The temperature is entered as °C.
- **Relative humidity (RH). %**

In the original adsorption isotherm there is no compensation for moisture. There is quite a lot of data in the literature regarding influence of moisture on the activated carbon capacity and we have designed a simple model for compensating the adsorption capacity for the presence of water in the air. In this model you can create a curve for how the water influences the capacity of the carbon in the case you are calculating. To the right of the chart "Capacity as function of RH" there are two cells where you can put in a break point (the value for RH when the capacity of the carbon starts to change) and the remaining capacity at 100 % RH. The model then compensates the adsorption capacity

according to this curve for the RH value you put in.

A general shape of this curve for many organic solvents is that the decrease in capacity starts at around 50 % RH and at 100 % RH around 20 % of the adsorption capacity for the solvent remains. **Note that this is a very rough estimation!**

Take special care when calculating for solvents that are water soluble (e.g. alcohol's).

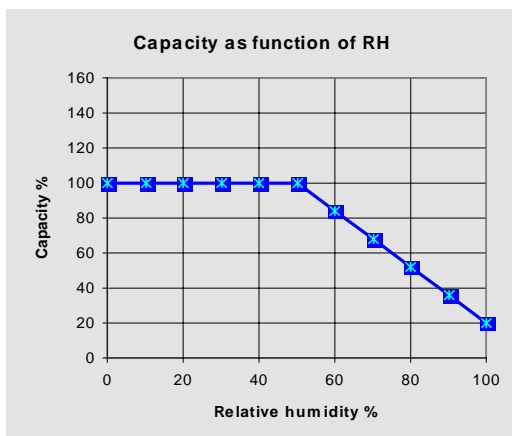


Fig. 1. The chart for the change in capacity as function of Relative Humidity. In this case the break point is set to 50 % RH and remaining capacity to 20 %.

- **Inlet concentration (C_1).** Also called challenge concentration.

Here we also enter the **breakthrough concentration**. It is not used for the W_e calculation but it is linked to the sheets with the breakthrough time calculations.

When all data is in place the Adsorption capacity is calculated and shown in the cells $W_{e \text{ original}}$ and $W_{e \text{ humidity compensated}}$.

There is also a chart with the adsorption isotherm curves for the concentration range 1 to 10 000 ppm to the right of the RH compensation chart.

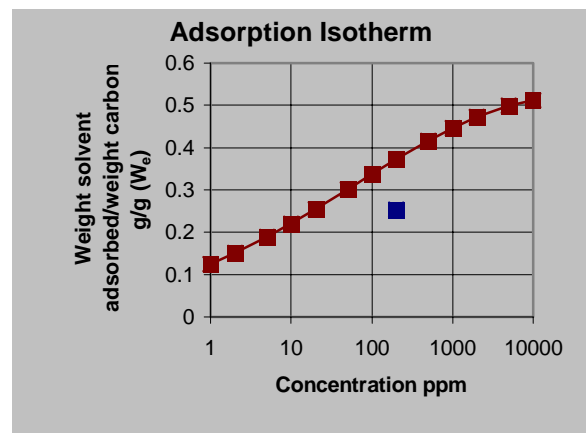


Fig. 2. The chart for the calculated adsorption isotherms.

Estimation of breakthrough time by calculation with the Mecklenburg equation

Now when we have a value for the adsorption capacity for the carbon/solvent combination we are working with, we can go on and make an estimation of the breakthrough time. This sheet contains a model for calculating the breakthrough time with the Mecklenburg equation. To do this calculation we need the following data.

- **Diffusion coefficient for the solvent (D).** This is a value for the spreading speed of the solvent.
- **External surface of the carbon (a_c).** This value can be obtained from the carbon suppliers or from literature. Normally this value is in the range 40 to 80 cm^2/g . The value is correlated to the void volume, density and granule diameter of the carbon.
- **Void volume in the carbon bed (V_v).** This is a value for how much empty space there is in the carbon bed. It does not include the micropores, and the value can be obtained from the carbon suppliers or

from literature. Normal values for the void volume are 0.3 to 0.5 cm³/g.

- **Carbon bulk density (ρ_c).** Can be obtained from carbon suppliers. It can also be easily measured.
- **Carbon granule diameter (d).** Can be obtained from carbon suppliers or measured. Entered in cm.
- **Height of carbon bed.** Entered in cm.
- **Diameter of carbon bed.** Entered in cm.
- **The number of filters in the mask (n).**
- **Air flow rate (Q).** Entered in l/minute.
- **Viscosity of upstream air (η).** This value is set to 1.83 E-04 g/cm^{-s} and normally it does not need to be altered.
- **Density of influent air (ρ_a).** This value is already in the model with correlation for changes in temperature. The value in the model is for 760 mmHg.

Remark. One reason for changing the viscosity and density values in the model could be if you are calculating with different air pressures. In that case new values for the air can be found in chemical and engineering handbooks.

- **Cross sectional area of the carbon bed (A).** This value is calculated from the diameter and no. of filters input above.
- **Carbon volume (V).** This is calculated from diameter, height and no. of filters entered above.
- **Molecule weight of solvent (M).**
- **Inlet concentration (C_I).**
- **Breakthrough concentration (C_b).**
- **Adsorption capacity (W_e).** Note that it is the humidity compensated value that is used.

When all data is in place you will get the breakthrough time in minutes and hours for the breakthrough concentration you have chosen. You also get the breakthrough curve for a range up to 2 times the breakthrough concentration.

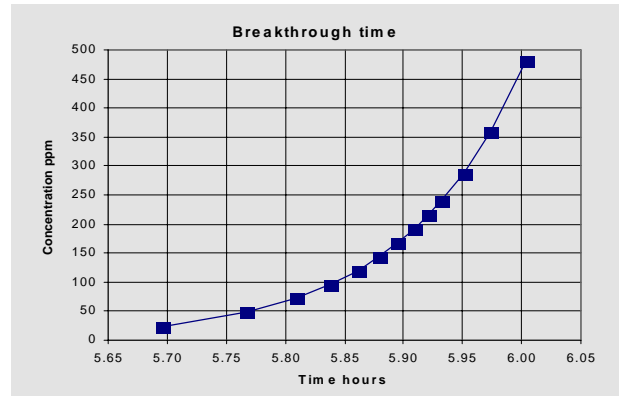


Fig. 3. Breakthrough curve from the Mecklenburg equation.

$$t_b = \frac{W_e \rho_c A n}{Q C_o} \left[z + \frac{1}{a_c \rho_c} \left(\frac{dG}{n} \right)^{0.41} \left(\frac{\eta}{\rho_a D_{20}} \right)^{0.67} \ln \left(\frac{C_b}{C_I} \right) \right]$$

Equation 2. The Mecklenburg equation

Estimation of breakthrough time by calculation with the Wheeler equation

To solve the Wheeler equation we need the the following data.

- **Inlet concentration weight / volume (W_o).** This value is calculated from molecular weight and inlet concentration volume / volume.
- **Flow rate (Q).**
- **Total weight of carbon (W_c).**
- **Carbon density (ρ_c).**
- **Inlet concentration volume / volume (C_I).**
- **Breakthrough concentration volume / volume (C_b).**
- **Molecular weight of solvent (M).**
- **Carbon granule diameter (d).**
- **Number of filters (n).**
- **Height of carbon bed.**
- **Diameter of carbon bed.**
- **Cross sectional area of carbon bed (A).** Calculated from the diameter.

- **Adsorption rate constant (k_v).** This **constant** describes the structure and the shape of the carbon bed in the equation. It is calculated from the data above.

$$k_v = 14.4 \left(\frac{1000Q}{nA} \right)^{1/2} d^{-3/2}$$

Equation 3. The Adsorption rate equation.

- **Adsorption capacity (W_e).** Note that it is the humidity compensated value that is used.

$$t_b = \frac{W_e}{C_o 1000Q} \left[W - \frac{\rho_c 1000Q}{k_v} \ln \left(\frac{C_I}{C} \right) \right]$$

Equation 4. The Wheeler equation.

When all data is in place you will get the breakthrough time in minutes and hours for the breakthrough concentration you have chosen. You also get the breakthrough curve for a range up to 2 times the breakthrough concentration.

Estimation of breakthrough time by calculation with the Yoon equation

This equation is solved with exactly the same data as the Wheeler equation. It is arranged in a slightly different way giving another shape of the breakthrough curve at high breakthrough concentrations.

$$t_b = \frac{W_e}{C_o 1000Q} \left[W - \frac{\rho_c 1000Q}{k_v} \ln \left(\frac{C_I - C}{C} \right) \right]$$

Equation 5. The Yoon equation

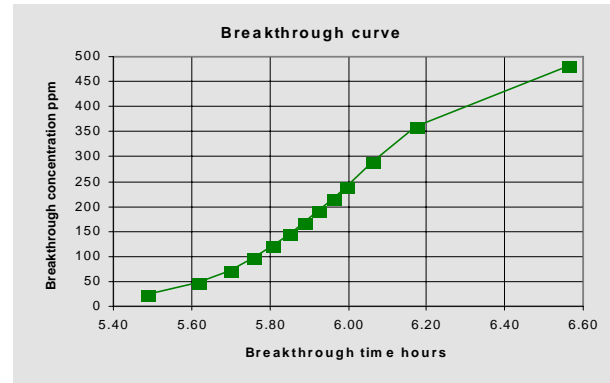


Fig. 4. The breakthrough curve calculated with the Yoon equation and 500 ppm inlet concentration.

Comparison of breakthrough curves from the different equations.

A chart is also created for comparison of the breakthrough curves for the different equations.

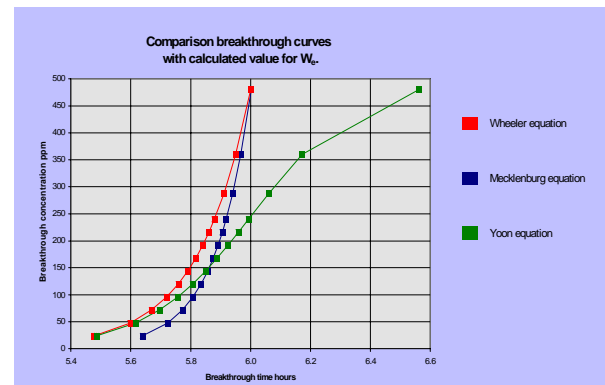


Fig. 5. Breakthrough curves for the Mecklenburg, Wheeler and Yoon equations.

Simplified estimation of breakthrough time when only the concentration is changed.

This is an easy way to estimate the change in breakthrough time when only the concentration is changed. The relation between concentration and breakthrough time is quite well known for many organic solvents. If no other parameters than the concentration are changed the new breakthrough time can be estimated with a simple equation.

What is interesting about this method is that there is data available for substances other than organic solvents.

You need to enter the following data.

- **The first concentration value.**
- **The breakthrough time at that concentration.**
- **The new concentration.**
- **A constant for the slope** of the curve describing the relation between concentration and breakthrough time for the substance you are working with.

The best way to get this constant is of course to test the filter at some different concentrations and calculate the slope from this data.

$$t_b = t_b' \left(\frac{C'}{C} \right)^b$$

Equation 6. Equation for estimating breakthrough time when changing concentration.

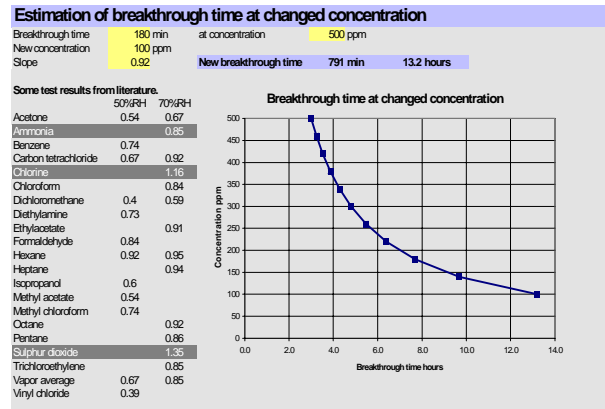


Fig. 8. On sheet 13 you can estimate a new breakthrough time if only concentration is changed and all other parameters influencing the breakthrough time are kept constant.

Once again, note that the condition for this calculation is that **no other parameters than the concentration are changed.**

If you have two test results for a filter with different concentration but all other parameters constant you can easily calculate the slope of the concentration / breakthrough time relationship with the iteration tools in Excel.

Conclusions

The general opinion about calculating the service life of gas filters seems to be that it is very difficult and that the result is very inaccurate. Neither of this needs to be true. A lot of material about this is published and the models are not more complicated than they can be handled in an ordinary PC spreadsheet program which also has the capacity to present the results on charts.

The accuracy is very much dependent on the input data. If we have test results to enter the accuracy will increase significantly.

Another reason for taking a look at these calculating models is that a new type of powered respirators are entering the market.

It will in a close future be possible to buy a RPE that measures the air volume that is passing through the filters and also will give the user a warning when a preset value is reached. This is probably just the beginning of a new generation of intelligent breathing protection equipment which will back up the users nose with a lot of powerful features

when it comes to making decision about when it is time to change filter.

Yet another reason is that it is becoming more and more obvious that some type of breathing protection program is needed to achieve a good protection level. In many applications these calculating models could be a valuable part of such a program.

Some examples of how the workbook can be used.

1. How long will filter XXX last when used in an environment containing 200 ppm toluene and 50 % RH in room temperature (we have no test results or other capacity values available)? It is quite demanding work and the minute air flow is estimated to be 40 l/min.

First we have to calculate the adsorption isotherm. This is done in sheet 1 and we have to enter the following values.

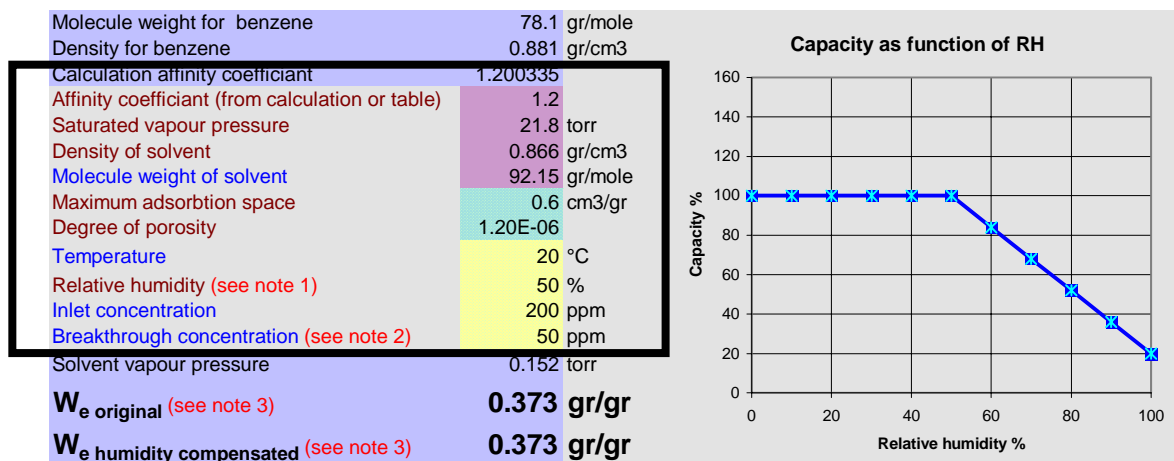


Fig 9.

As the RH was so low there is no difference between the two values for W_e . The value on the last row is linked to the next sheet. There we have to enter some more data.

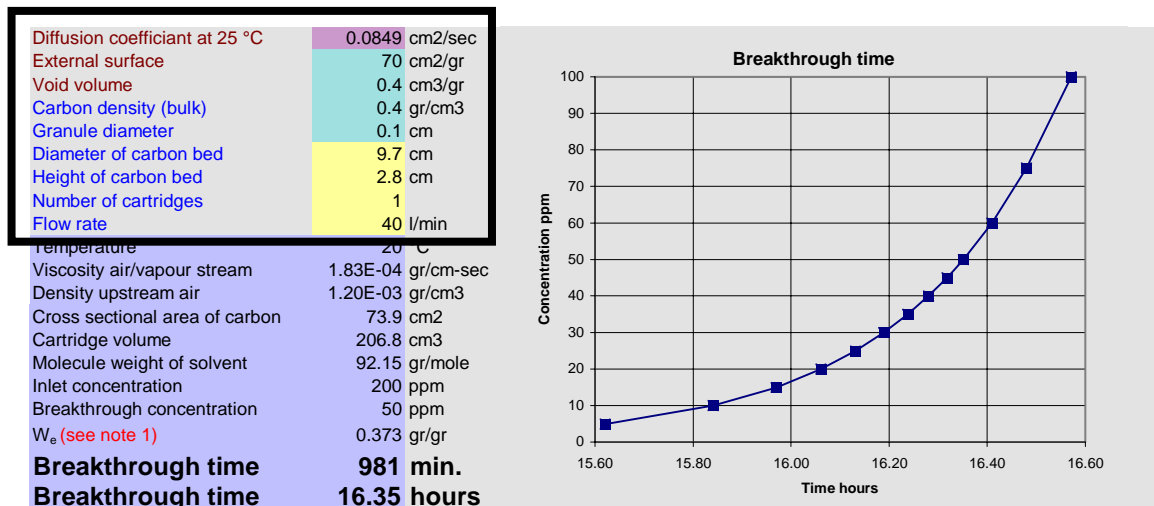


Fig. 10

At the same time the breakthrough time is calculated in sheet 3 and 4 with the other equations and the result is shown on sheet 5. The curves for all three equations are quite equal and the **breakthrough time is around 16 hours.**

Note that the parameters on the first 3 rows only are used on this sheet. The other two equations will be solved without these data.

2. How long will this filter last if the temperature rises to 25 °C and the RH to 80 % ?

Toluene is an aromatic solvent and it is not soluble in water. No test results could be found for toluene in conjunction with high humidity. It is however very reasonable to assume that toluene acts in the same way as its close relative benzene and many other organic solvents. Test results for benzene were found and they showed that apr. 60 % of the capacity remained at 80 % RH, and had hardly any influence below 50 % RH.

We begin by adjusting the humidity compensating curve to these results. This is achieved by setting the break point to 50 % and remaining capacity at 100 % RH to 30 %.

Then we enter the new temperature and the relative humidity values.

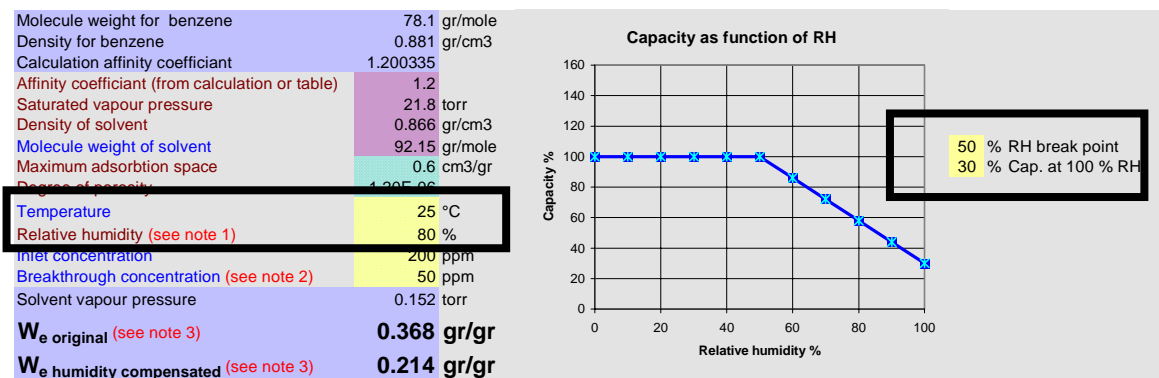


Fig. 11

We now have a new value for W_e which is linked to sheets 2, 3 and 4.

No more data input is needed. A new breakthrough time is calculated with all three equations and the result is shown on each sheet and on sheet 5. **The breakthrough time decreased to around 9 hours.**

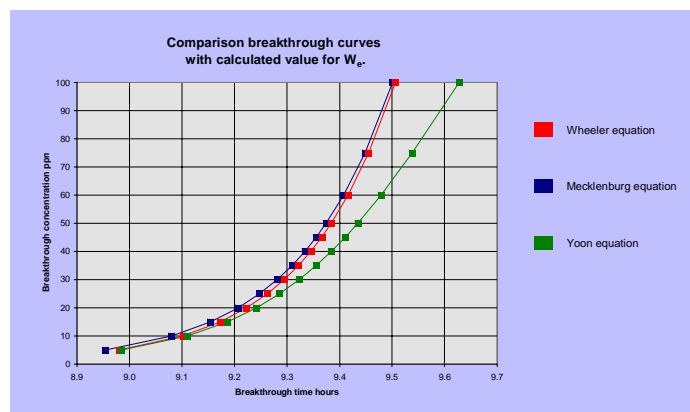


Fig. 12. Breakthrough curves for the calculation above.

3. What happens if we change the toluene to the less volatile xylen in the application?

If we change the values related to the solvent we will see that **the breakthrough time will change very little. It increases to around 17 hours.**

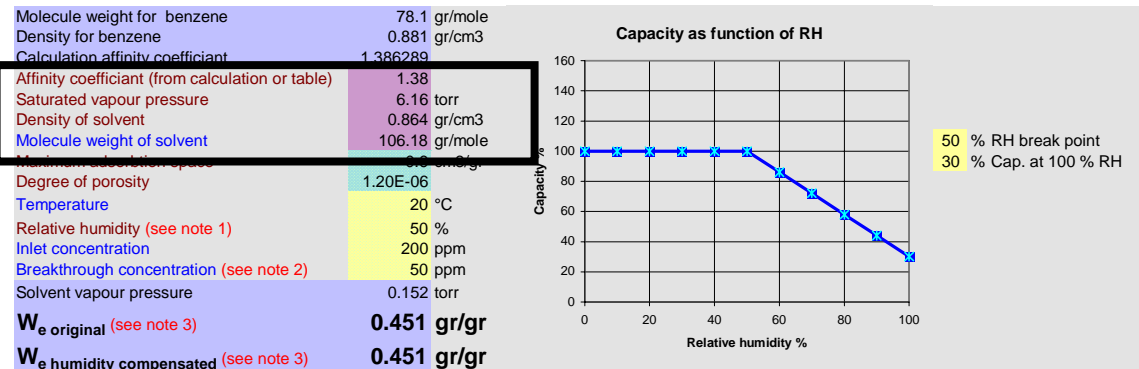


Fig 13.

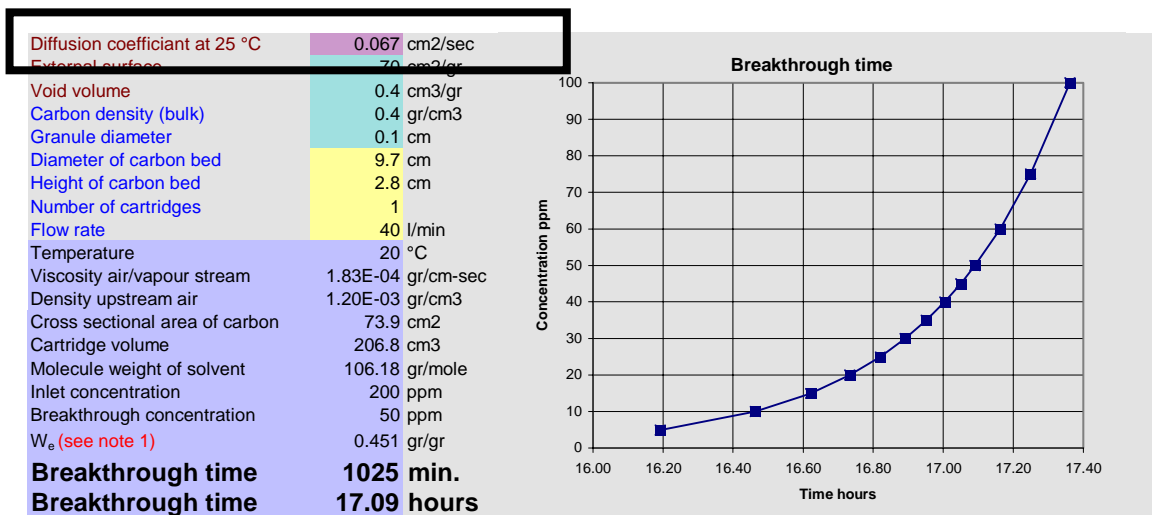


Fig. 14.

Remark. In practice the concentration probably will decrease because of the lower volatility. If the concentration is decreased to 150 ppm the breakthrough time will increase to around 22 hours in dry atmosphere and around 13 hours in hot and humid environment.

4. How long will filter XXX last against 250 ppm styrene at 22 °C and 50 % RH ?

First we fill in chemical data and the user conditions. We can't find any test results regarding the humidity but styrene is an aromatic organic solvent so we assume it behaves in the same way as e.g. benzene, that is a quite large decrease in capacity in presence of water. As styrene is slightly water soluble we set the break point for the humidity compensation curve to 40 % and the remaining capacity at 100 % RH to 20 %.

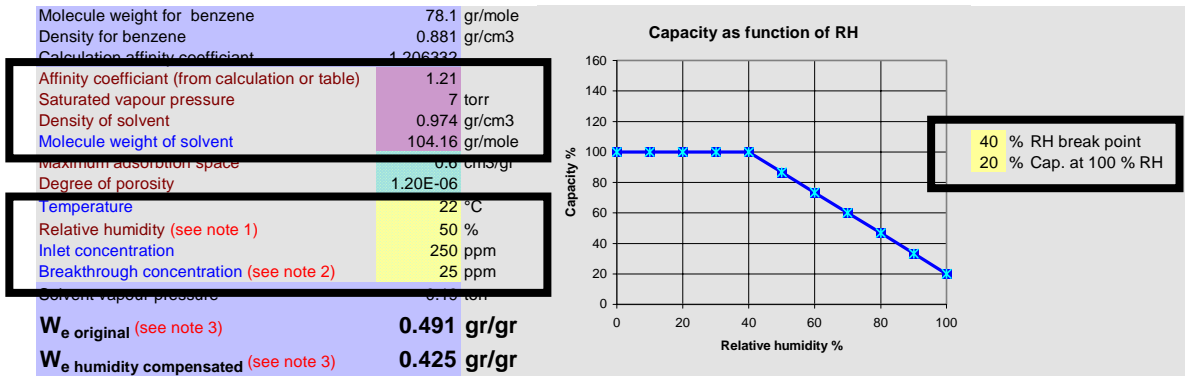


Fig. 15.

The workload in this case is not particularly hard so we set the air flow to 30 l/min. We can't find any value for the diffusion coefficient which means the Mecklenburg equation cannot be solved. We have to go to sheet 2 to enter the data necessary for solving the Wheeler and Yoon equations.

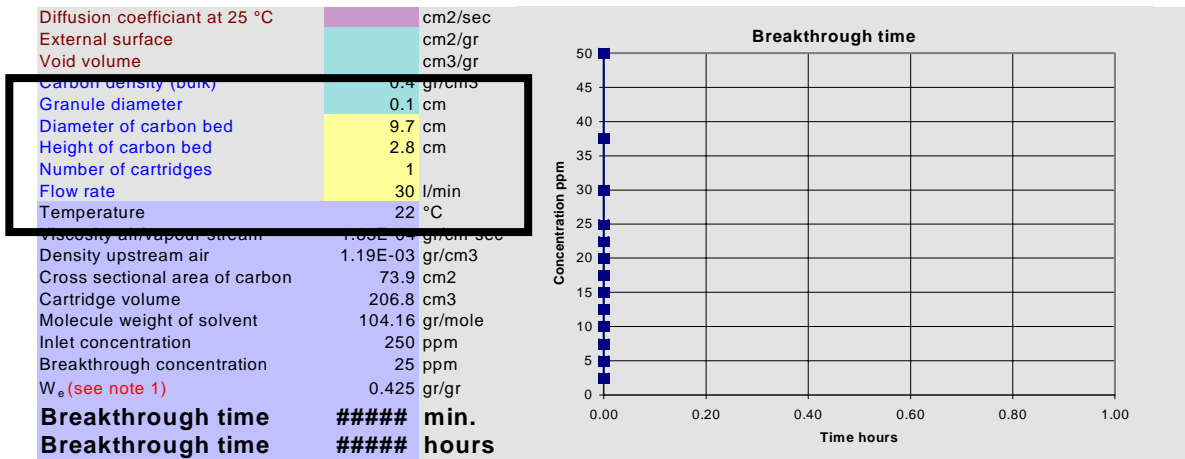


Fig. 16.

After this is done we can go to sheet 3 and 4 and check the result for the breakthrough time.

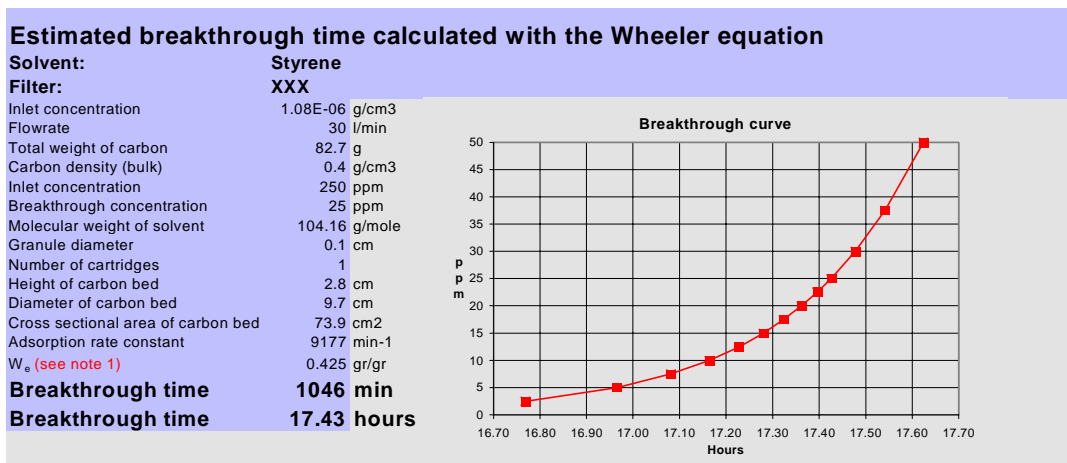


Fig. 17

The breakthrough time is very similar with these equations, **around 17 hours** in this case.

5. The filter supplier has another smaller filter with same type of carbon. It has slightly larger granules (1.5 mm) and is 2.1 cm high. This gives a lighter filter with lower breathing resistance. It is also cheaper.

The filters have so far been changed every second day. How much must we change the concentration if we shall keep this routine with the smaller filter?

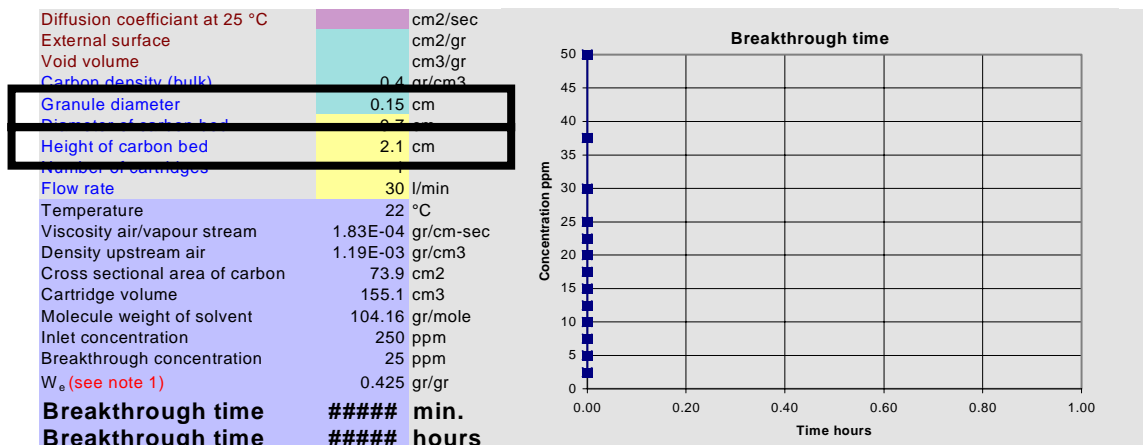


Fig. 18.

Begin by adding the new filter parameters on sheet 2. Then let Goal Seek do the job for you.

- Go to the desired equation on sheet 3 or 4.
- Place the marker in the breakthrough time cell.
- Open Goal Seek (Tools menu).
- Write in your desired value e.g. 17.5 hours.
- Place the marker in square “By changing cell”, open sheet 1 and click on the cell for inlet concentration value.

Now the adsorption capacity and breakthrough time are calculated until the target value is reached.

Result: If we lower the concentration to 170 ppm we can use the new smaller filter as long as the existing one at 250 ppm.

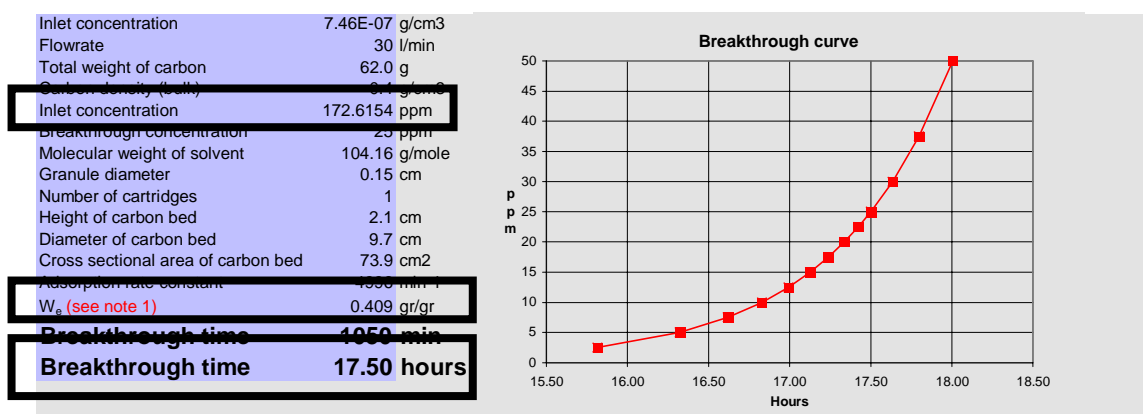


Fig. 19.

Note that when the concentration is changed the adsorption capacity is also recalculated to a lower value.

- An E1-filter is tested against sulphur dioxide in 500 ppm concentration and 70 % RH. All the other parameters were adequate for this work place. What service life can we expect using the filter in 50 ppm concentration and 70 % RH if the breakthrough time at 500 ppm was 130 minutes?

This can be estimated on sheet 13. Tests have shown that the slope constant 1.35 is relevant in the whole range from 100 to 5000 ppm. It is then fully reasonable to assume that the curve can be extrapolated to 50 ppm.

Enter your test results in the first two input cells. Then enter your new concentration and the slope for the relation between the two concentrations.

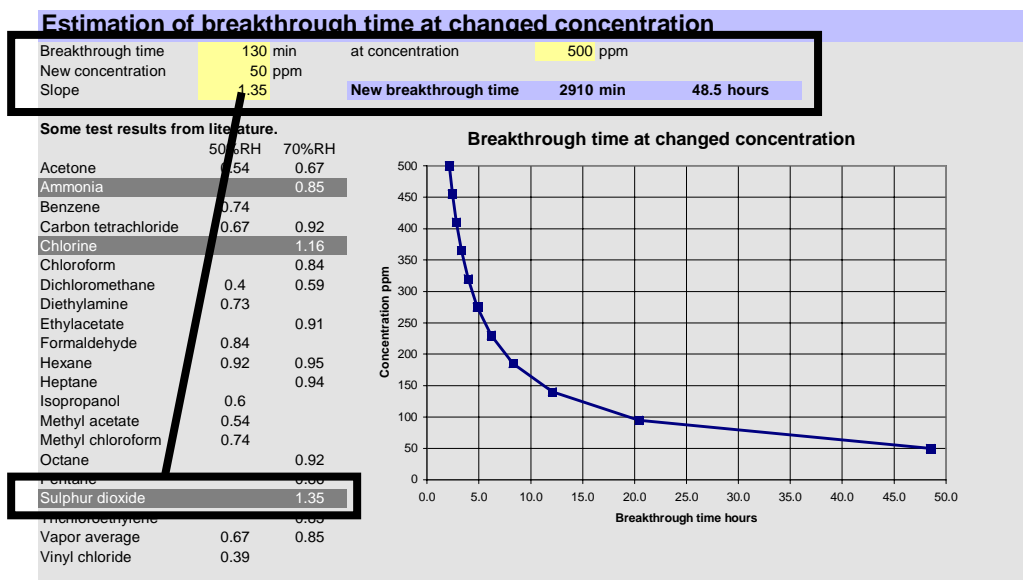


Fig. 20

You will now get the calculated breakthrough time for your input concentration and a breakthrough time curve for the whole range between your two concentration values. **You can expect a service life of around 48 hours in 50 ppm concentration.**

Note that a requirement for this calculation is that no other parameter than the concentration is changed.

- Hexane is used in a workplace and the filter is changed when breakthrough is detected by smell. This normally occurs after 8 hours work. The concentration is measured to be 500 ppm and very steady. The work is done in normal room temperature and the humidity is low. A new worker is employed and he claims that his filter has expired after 5 hours. What might be the reason for this difference?

All parameters in the workplace are well measured and documented. The only thing that is not investigated is the workload and air consumption. Is it really possible that the air flow differs that much between two persons? Lets take a look at the air flows in this case.

Start by estimating the filter capacity for Hexane. This is done on sheet 1 and when all data is entered we have the following result.

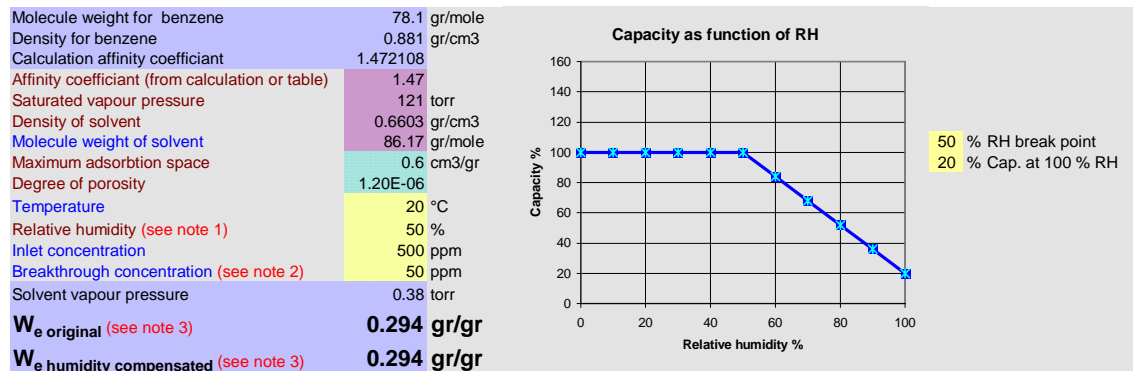


Fig. 21.

Now go to sheet 2, enter the rest of the data and let Goal Seek do the job.

- Place marker in the cell for the breakthrough time.
- Open Goal Seek.
- Fill in the target value for one of the workers (e.g. 8 h)
- Place the marker at “By changing cell”.
- Click at the flow rate cell.

This gives the result that the air flow in this case was 27 l/min. Now make the same operation for the other worker. The result this time is an air flow at 43 l/min.

Is this correct?. Can two persons doing the same work in the same environment have such different air consumption? The answer is yes. Measurement on people have shown that this is absolutely normal and must be taken into consideration when estimating service life for filters. In fact, even larger differences than this have been recorded.

8. *We have a filter with very little data regarding the carbon and we can't get any more information from the supplier. All we have is a capacity value for carbon tetrachloride, and the W_e value for the filter is 0.600 g CCl_4 / g carbon at 1000 ppm and 50 % RH. How can we apply these data to other solvents?*

What we have to do is to fit the available test result to an adsorption isotherm curve. This can be done on sheet 6. We enter all necessary data for CCl_4 and the test conditions. The carbon parameters needed here are the maximum adsorption space and the degree of porosity. These are interrelated and we have made rough correlation for a number of different carbons on sheet 17.

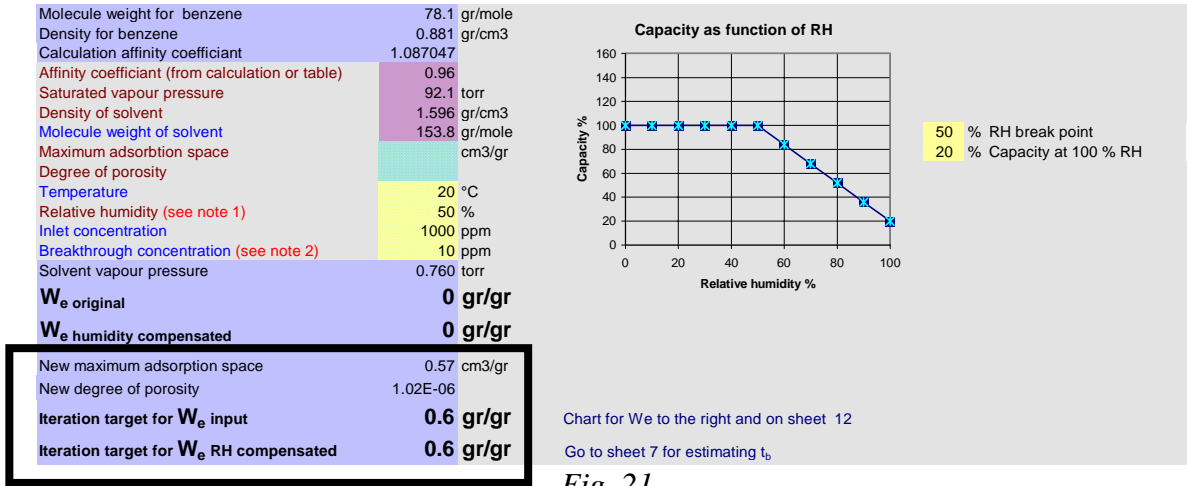


Fig. 21.

As you see on sheet 6 we have some extra rows with these carbon values and for W_e . The maximum adsorption space and the degree of porosity is interrelated with the correlation factor from sheet 17.

- Place the marker in one of the W_e cells and open Goal Seek.
- Enter your target value, in this case 0.600 g/g.
- Place marker in square “By changing cell”.
- Click on the cell for “New maximum adsorption space”.

New values are calculated for the carbon and an adsorption isotherm curve is shown to the right.

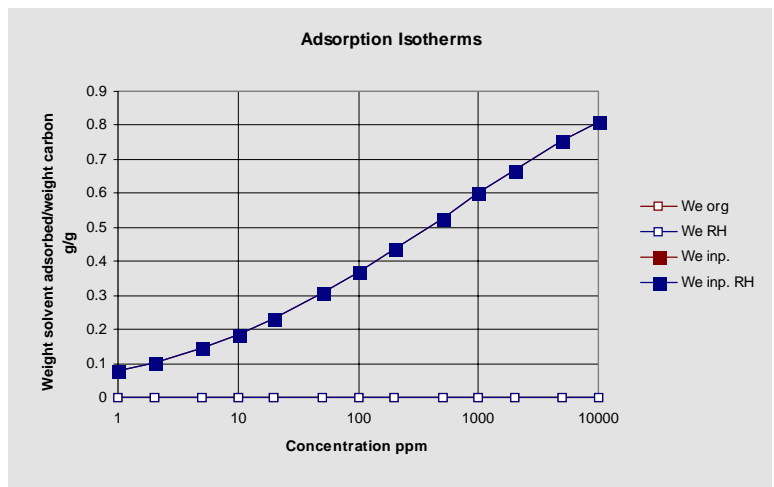


Fig. 22.

Now we can enter your carbon structural values in their ordinary locations on the sheet and estimate filter capacity for other solvents and/or conditions.

Note that the correlation to maximum adsorption space is based on a quite small amount of number, so breakthrough values based on this isotherm will be less certain.

In order to make a breakthrough time calculation from this we must of course have some other carbon values, but in order to solve the Wheeler and Yoon equations we need only density and granule size, and they can be measured quite easily.

Definitions of some terms relating to activated carbon

Absorption

A process in which fluid molecules are taken up by a liquid or solid and distributed throughout the body of that liquid or solid.

Activated carbon

A family of carbonaceous substances manufactured by processes that develop adsorptive properties.

Adsorbate

Any substance that is or can be adsorbed.

Adsorbent

Any solid having the ability to concentrate significant quantities of other substances on its surface.

Adsorption

A process in which fluid molecules are concentrated on the surface by chemical or physical forces, or both.

Chemisorption (chemical adsorption)

The binding of an adsorbate to the surface of a solid by forces whose energy levels approximate those of a chemical bond.

Density, apparent (density, bulk)

The weight under specified conditions of a unit volume of an activated carbon including its pore volume and inter-particle voids.

Desorption

Separation of an adsorbate as such from activated carbon.

Equilibrium adsorptive capacity

The quantity of a given component adsorbed per unit of activated carbon from a fluid or fluid mixture at equilibrium temperature and concentration or pressure.

Isotherm

A plot of quantity adsorbed per unit of activated carbon against equilibrium concentration, or pressure, when temperature is held constant.

Macropore

A pore in activated carbon having a diameter greater than 5000 Å.

Micropore

A pore in activated carbon having a diameter less than 40 Å.

Physical adsorption (van der Waals adsorption)

The binding of an adsorbate to the surface of a solid by forces whose energy levels approximate those of condensation.

Pores

The complex network of channels in the interior of a particle of activated carbon.

Pore volume

Volume of the pores in a unit weight of activated carbon.

Retentivity

The ability of an activated carbon to resist desorption of an adsorbate.

Service life (service time)

The elapsed time until the end point is reached in an adsorption process.

Sorption

A process in which fluid molecules are taken up by absorption and adsorption.

Transitional pore

A pore in activated carbon having a diameter between 40 and 5000 Å.

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