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# INCREASING THE PROTECTIVE EFFECT OF THE RESPIRATOR ON CHEMICALLY BOUND OXYGEN

EKHILEVSKIY STEPAN GRIGORIEVICH,
GOLUBEVA OKSANA VALERIEVNA,
ZABELENDIK OLGA NIKOLAEVNA
Euphrosyne Polotskaya State University of Polotsk

**Аннотация:** Для оптимизации респиратора на химически связанном кислороде развит формализм моделирования регенерации воздуха слоем гранул надпероксида калия, диаметр которых меняется в направлении фильтрации. Показано, что в изолирующем аппарате (работающем по круговой схеме) прирост по времени критического проскока, вызванный четырьмя скачками диаметра гранул, составит 25,9% и будет равен приросту связанного углерода в открытой схеме.
**Ключевые слова:** респиратор, динамика сорбции, надпероксид калия, работающий слой хемосорбента, размер гранул.

**УВЕЛИЧЕНИЕ ЗАЩИТНОГО ДЕЙСТВИЯ РЕСПИРАТОРА НА ХИМИЧЕСКИ СВЯЗАННОМ КИСЛОРОДЕ**

**Ехилевский Степан Григорьевич,**
**Голубева Оксана Валерьевна,**
**Забелендик Ольга Николаевна**

**Abstract:** To optimize a respirator on chemically bound oxygen, a formalism has been developed for modeling air regeneration by a layer of potassium superoxide granules, the diameter of which changes in the direction of filtration. It is shown that in an insulating apparatus operating in a circular circuit, the increase in time of the critical breakthrough caused by four jumps in the diameter of the granules will be 25.9% and will be equal to the increase in bound carbon in an open circuit.
**Key words:** respirator, sorption dynamics, potassium superoxide, working layer of chemisorbent, granule size.

**Reasons for the inefficient use of the protective resource of the respiratory organs on chemically bound oxygen**

Being an insulating means of protection, the breathing apparatus has a closed circuit of the airway part. This means that the exhaled air regenerated in the process of filtration through the oxygen-containing product is returned to the inhalation. Human poisoning with carbon dioxide begins when its content in the inhaled air exceeds 1.5% [1]. By the time of such a (critical) breakthrough of $CO_2$ through the regenerative cartridge, the layers of the oxygen-containing product (especially the trailing ones) have not been completely developed. Otherwise, the $CO_2$ slip would be 4%. An integral characteristic of the unused resource of the regenerative cartridge is the width of the dead layer of the sorbent formed from potassium superoxide molecules that have not reacted by the end of the protective action of the apparatus (the moment of critical breakthrough of $CO_2$ through the regenerative cartridge). This width depends on the mode in which the breathing apparatus was operated (volume air flow) and the characteristics of the oxygen-containing product that determine the chemisorption kinetics, which is generally characterized by the dimensionless length of the regenerative cartridge $\eta$ [2]. At the beginning of the operation of the apparatus (until the layer-by-layer development of the absorption resource of the chemisorbent has begun), a decrease in the proportion of $CO_2$ molecules in a given sorbent layer does not depend on its distance from the cartridge inlet and is determined only by the thickness of this layer and the concentration pressure of $CO_2$ at its inlet. This provides an exponential decline in carbon dioxide concentration with distance from the entrance to the cartridge. In particular, if $\eta < 0{,}98$ the $CO_2$ breakthrough from the very beginning exceeds the critical breakthrough ($e^{-\eta} > 1{,}5/4$), and the share of the used protective resource (the degree of its depletion) is equal to zero (the entire chemisorbent layer is dead). Thus, the lower efficiency of using the protective resource in breathing apparatus designed for a short period of protective action is confirmed.

The second reason for the inefficient use of the protective resource of a regenerative cartridge is the sintering of granules of an oxygen-containing product under the action of exothermic heat released during chemisorption

$$4KO_2 + 2CO_2 = 2K_2CO_3 + 3O_2 + 360kJ. \quad (1)$$

The density of its sources is the higher, the thinner the working layer of the sorbent. Its width (with the given characteristics of chemisorbent granules) is determined by the volume flow rate of air (the rate of its filtration), the value of the concentration pressure and the degree of depletion of the absorption resource. For these reasons, the width of the working layer of the sorbent increases as it moves deeper into the cartridge [3]. This means that the maximum thermal power is realized in the frontal layer of the chemisorbent at the beginning of the operation of the breathing apparatus with a uniformly loaded regenerative cartridge.

**Mathematical model of $CO_2$ chemisorption by an in homogeneously equipped regenerative cartridge with an open scheme of the airway part**

Let us choose as a characteristic scale of the volumetric concentration of $CO_2$ molecules $W$ its maximum value $W_0$ at the entrance to the considered chemisorbent layer, which is achieved after the previous layer has been completely exhausted. If we neglect the return of the $CO_2$ breakthrough to inhalation (to simulate the working process in a regenerative cartridge connected according to an open circuit), $W_0$ coincides with the value of $W$ in the exhaled air. In such a situation, the reduced concentration of $CO_2$ $\omega = W / W_0$ molecules, according to [4], is determined by the relations

$$\xi(x) = \beta x / v, \qquad \tau(t) = \beta\gamma t, \quad (2)$$

$$\omega(\xi,\tau) = e^{-\xi-\tau}\sum_{k=0}^{\infty}\frac{f_k(\tau)}{k!}\xi^k, \quad (3)$$

$$f_{k+1}(\tau) = \int_0^{\tau} f_k(\tau)\,d\tau, \quad (4)$$

$$f_0(\tau) = e^{\tau}\omega(0,\tau), \quad (5)$$

$$u(\xi,\tau) = e^{-\tau}\int_0^{\tau} e^{\tau}\omega(\xi,\tau)\,d\tau, \quad (6)$$

where $\xi$ and $\tau$ are the dimensionless coordinate ($\xi \in [0, \eta]$) and the time corresponding to the real time of the filter operation $t$, and the distance $x$ from the entrance to the absorbing layer, $v$ are the air filtration rate, $\beta$ and $\gamma$ phenomenological constants characterizing the rate of chemisorption and its resource in a cartridge uniformly equipped with granules of medium diameter [5, 6], $u$ is the used fraction of the absorption resource of the chemisorbent.

Assuming that the level of physical activity of a person does not change and a constant concentration of $CO_2$ ($\omega(0,\tau) = 1$) enters the regenerative cartridge, we find the solution of the recurrence relation (4), (5)

$$f_k(\tau) = f_{0;k}(\tau) = e^{\tau} - \sum_{l=0}^{k-1}\frac{\tau^l}{l!}, \quad (7)$$

where index is 0; indicates the number of jumps in the diameter of the granules of the oxygen-containing product in the direction of exhaled air filtration. Substituting the result into (3), we obtain the reduced $CO_2$ concentration

$$\omega_0(\xi,\tau)=e^{-\xi}\left[1+\sum_{n=1}^{\infty}\frac{\xi^n}{n!}\left(1-e^{-\tau}\sum_{k=0}^{n-1}\frac{\tau^k}{k!}\right)\right], \tag{8}$$

and then, using (6), the fraction of spent chemisorbent in the cartridge without a jump in the diameter of the granules

$$u_0(\xi,\tau)=1-e^{-\tau}\left(1+e^{-\xi}\sum_{n=1}^{\infty}\frac{\xi^n}{n!}\sum_{k=1}^{n}\frac{\tau^k}{k!}\right). \tag{9}$$

To prevent sintering, let us place oversized granules 5 mm in diameter in the frontal layer of the chemisorbent ( $\xi\in[0,\zeta_1]$ ). In this case, *β* in (2) must be replaced by $\alpha_1\beta$, where, in accordance with the previously stated $a_1=16/25$ (equal to the square of the ratio of the previous (average) diameter of the granules, they occur in the frontal part of the cartridge (before the first diameter jump) [7]. As a result, using (2) – (8) we get the Heaviside function *θ*

$$\omega_1(\xi,\tau)=\omega_0(\alpha_1\xi,\alpha_1\tau)\theta(\zeta_1-\xi)+\omega_{12}(\xi-\zeta_1,\tau)\theta(\xi-\zeta_1), \tag{10}$$

$$u_1(\xi,\tau)=u_0(\alpha_1\xi,\alpha_1\tau)\theta(\zeta_1-\xi)+u_{12}(\xi-\zeta_1,\tau)\theta(\xi-\zeta_1), \tag{11}$$

where in order to absorb $CO_2$ $\omega_{12}$ and work out the chemisorbent $u_{12}$ in the second (equipped with 4 mm granules) part of the cartridge in (3), (6) $\xi$ should be replaced by $\xi-\zeta_1$, in (5) instead of $\omega(0,\tau)$ substitute $\omega_0(\alpha_1\zeta_1,\alpha_1\tau)$, and in (6) instead of $\omega$ expressions for $\omega_{12}$. The first index indicates the number of jumps in the diameter of the granules, the second – the number of the part of the cartridge.

The coordinate of the jump in the diameter of the granules $\zeta_1=0{,}681$ is chosen from the condition of equality of the derivatives $\partial u_1(0,\tau)/\partial\tau\big|_{\tau=0}=\partial u_1(\zeta_1+0,\tau)/\partial\tau\big|_{\tau=0}=0{,}64$ proportional to the power of the sources of exothermic heat at the inlet to the first and second parts of the cartridge at the initial moment of time. It is important that in an uncut cartridge $\partial u_0(0,\tau)/\partial\tau\big|_{\tau=0}=1$, i.e., an increase by 1 mm in the diameter of the granules in the frontal layer of the chemisorbent by 36% reduces the density of the maximum power of exothermic heat sources in the regenerative cartridge, preventing sintering of the oxygen-containing product.

Similarly (from the condition of equal power of exothermic heat sources at the entrance to the second and third parts of the regenerative cartridge), the dimensionless coordinate $\zeta_2=1.249$ of the second jump in the diameter of the granules ( $\beta\to\alpha_3\beta$ ) from 4 to 3 millimeters ( $\alpha_3=16/9$ ) was determined, for which the following from (2) – (6) were used formulas

$$\omega_2(\xi,\tau)=\omega_1(\xi,\tau)\theta(\zeta_2-\xi)+\omega_{23}(\xi-\zeta_2,\tau)\theta(\xi-\zeta_2), \tag{12}$$

$$u_2(\xi,\tau)=u_1(\xi,\tau)\theta(\zeta_2-\xi)+u_{23}(\xi-\zeta_2,\tau)\theta(\xi-\zeta_2), \tag{13}$$

in which

$$\omega_{23}(\xi,\tau)=e^{-\alpha_3(\xi+\tau)}\sum_{k=0}^{\infty}\frac{f_{2;k}(\tau)}{k!}(\alpha_3\xi)^k, \tag{14}$$

$$f_{2;0}(\tau)=e^{\alpha_3\tau}\omega_1(\zeta_2,\tau),\qquad f_{2;k+1}(\tau)=\alpha_3\int_0^{\tau}f_{2;k}(\tau)d\tau, \tag{15}$$

$$u_{23}(\xi,\tau)=e^{-\alpha_3\tau}\alpha_3\int_0^{\tau}e^{\alpha_3\tau}\omega_{23}(\xi,\tau)d\tau. \tag{16}$$

The dimensionless coordinates $\zeta_3=1.693$ and $\zeta_4=2.0093$ of both the third (from 3 to 2 mm) and the fourth (from 2 to 1 mm) jumps in the diameter of the granules are found from the condition of the same power of the exothermic heat sources at the inlet to all (differing in the size of the granules) parts of the regenerative cartridge. Why were similar (12)-(16) formulas

$$\omega_n(\xi,\tau)=\omega_{n-1}(\xi,\tau)\theta(\zeta_n-\xi)+\omega_{n\,n+1}(\xi-\zeta_n,\tau)\theta(\xi-\zeta_n)\,, \tag{17}$$

$$u_n(\xi,\tau)=u_{n-1}(\xi,\tau)\theta(\zeta_n-\xi)+u_{n\,n+1}(\xi-\zeta_n,\tau)\theta(\xi-\zeta_n)\,, \tag{18}$$

$$\omega_{n\,n+1}(\xi,\tau)=e^{-\alpha_{n+1}(\xi+\tau)}\sum_{k=0}^{\infty}\frac{f_{n;\,k}(\tau)}{k!}(\alpha_{n+1}\xi)^k\,, \tag{19}$$

$$f_{n;\,0}(\tau)=e^{\alpha_{n+1}\tau}\omega_{n-1}(\zeta_n,\tau)\,,\qquad f_{n;\,k+1}(\tau)=\alpha_{n+1}\int_0^{\tau}f_{n;\,k}(\tau)d\tau\,, \tag{20}$$

$$u_{n\,n+1}(\xi,\tau)=e^{-\alpha_{n+1}\tau}\alpha_{n+1}\int_0^{\tau}e^{\alpha_{n+1}\tau}\omega_{n\,n+1}(\xi,\tau)d\tau\,, \tag{21}$$

in which $n=3,4,\ldots$ ($\alpha_4=16/4=4$ and $\alpha_5=16/1=16$).

**Modeling of a self-contained breathing apparatus with a circular scheme of the airway part**

In a device with a circular scheme of the airway part, a $CO_2$ slippage is added to the constant component specified by the operating mode of the device, monotonously increasing as the resource of the regenerative cartridge is exhausted. As a result, a self-consistent problem arises of determining the desired function $\overline{\omega}(\xi,\tau)$, where the overline denotes the closeness of the airway part. To solve the self-consistent problem, we used an iterative procedure with a small parameter $\overline{\omega}(\eta,\tau)$, where $\eta$ is the dimensionless cartridge length.

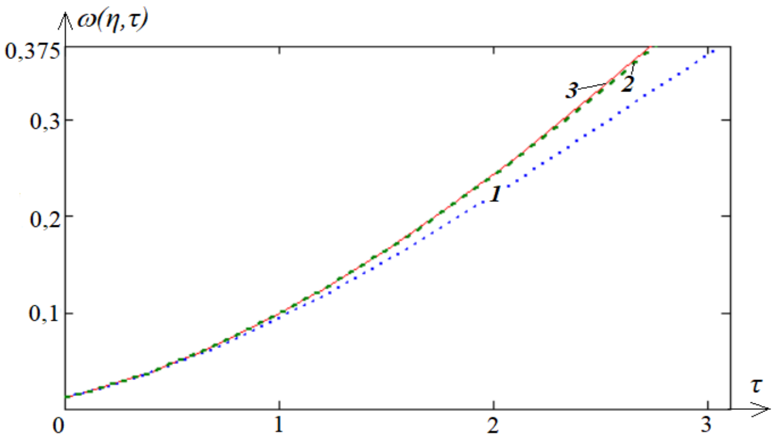
In the zeroth approximation ($\overline{\omega}(\xi,\tau)\approx\overline{\omega}_0(\xi,\tau)$), the slip should be neglected altogether. In this case, we return to the stationary boundary condition $\overline{\omega}_0(0,\tau)=1$, for which the solution of the recurrence relation (4) can be written in an analytical form (see (7)). Substituting (7) into (3), we obtain the well-known result $\overline{\omega}_0(\xi,\tau)=\omega(\xi,\tau)$ (see (8)).

The next step of the iterative procedure, corresponding to the first approximation ($\overline{\omega}(\xi,\tau)\approx\overline{\omega}_1(\xi,\tau)$), consists in substituting (8) into (22)

$$\overline{\omega}_1(0,\tau)=1+\omega(\eta,\tau)\,, \tag{22}$$

and numerical implementation of the recurrent procedure (4). Its results are presented graphically in Fig. 1 (curve 2).

It can be seen that at the beginning, when the $CO_2$ slippage is insignificant, the dependences plotted for the open (curve 1) and circular patterns (curve 2) of the air duct part practically do not differ. However, as the cartridge resource is exhausted, the slip in the circular pattern grows more rapidly, as it should be, because the $CO_2$ molecules that escaped chemisorption return to inhalation, increasing the carbon dioxide content in exhalation. Developing in the indicated direction, the process moves further and further away from what is taking place in the open




1 – according to the open circuit; 2 – in a circular pattern (first approximation), 3 – in a circular pattern (second approximation)

**Fig. 1. Evolution of $CO_2$ slip through the regenerative cartridge of a breathing apparatus on chemically bound oxygen, connected in a circular pattern.**

scheme. As a result, the time $\tau_k$ for the critical breakthrough of $CO_2$ is reduced by 9.8%.

The second iteration (corresponding to the approximation $\bar{\omega}_2(\xi,\tau)$) consists in substituting $\bar{\omega}_1(\eta,\tau)$ into (22) instead of $\omega(\eta,\tau)$. As a result, the $CO_2$ critical breakthrough time has decreased by another 0.7%, which is barely distinguishable. Therefore, curve 3, which corresponds to the second step of the iterative procedure, practically coincides with curve 2.

Let us discuss the issue of the convergence of the iterative procedure used in the actual range of change in the breakthrough. The physiology of respiration is such that carbon dioxide poisoning begins when its content in the inhaled air reaches 1.5%. Under normal conditions, a person exhales air with 4% carbon dioxide content. That is, the condition for the critical breakthrough of $CO_2$ has the form

$$\omega(\eta,\tau_\kappa)=1{,}5/4=0{,}375. \qquad (23)$$

This means that for $\tau \le \tau_\kappa$ the corrections to $\bar{\omega}_1(0,\tau)$ (see (22)) arising during the iterative procedure, they can be uniformly estimated by the terms of a decreasing geometric progression with the denominator $q=0{,}375$. The latter, as is known, converges at $q<1$.

**A quantitative measure of the increase in the protective effect due to a decrease in the diameter of the granules of an oxygen-containing product in the direction of exhaled air filtration**

In the same way as it was done in the previous paragraph, we can take into account the effect of the closeness of the airway part for a cartridge with four jumps in the diameter of the granules. In this case, expressions (17)-(19) for $n=4$ describing the slip of $CO_2$ through an in homogeneously loaded cartridge with four cuts, connected according to an open circuit, should be taken as the zero approximation of the iterative procedure. Since the slip through a non-uniformly loaded cartridge is less than through a homogeneous one, the second step of the iterative procedure is definitely not needed. So, there is no need to index these steps. Therefore, the boundary condition at the entrance to the first part of the in homogeneously loaded cartridge takes the form

$$\tilde{\omega}_{11}(0,\tau)=1+\omega_4(\eta,\tau), \qquad (24)$$

where the first index $\tilde{\omega}$ is the number of jumps in the diameter of the granules, the second is the number of the part of the cartridge, and the wavy line on top, in contrast to the straight line, reflects the heterogeneity of the cartridge with a circular scheme of the airway part.

Taking into account (24), relations (3) – (5) will take the form (25), (26)

$$f_{1;0}(\tau)=(1+\omega_4(\eta,\tau))e^{\alpha_1\tau}, \qquad f_{1;k+1}(\tau)=\alpha_1\int_0^\tau f_{1;k}(\tau)d\tau, \qquad (25)$$

$$\tilde{\omega}_{11}(\xi,\tau)=e^{-\alpha_1(\xi+\tau)}\sum_{k=0}^{\infty}\frac{f_{1;k}(\tau)}{k!}(\alpha_1\xi)^k, \qquad (26)$$

where the first index *f* is the number of the part of the cartridge, the second is the number of the step of the iterative procedure.

At the entrance to the second part of the in homogeneously loaded cartridge, a slip through its first part is received. Therefore, by analogy with (25), (26) we can write

$$f_{2;0}(\tau)=\tilde{\omega}_{11}(\xi_1,\tau)e^{\alpha_2\tau}, \qquad f_{2;k+1}(\tau)=\alpha_2\int_0^\tau f_{2;k}(\tau)d\tau, \qquad (27)$$

$$\tilde{\omega}_{12}(\xi,\tau)=e^{-\alpha_2(\xi+\tau)}\sum_{k=0}^{\infty}\frac{f_{2;k}(\tau)}{k!}(\alpha_2\xi)^k. \qquad (28)$$

Then for an in homogeneously loaded cartridge with one jump in the diameter of the granules with a circular connection scheme, we obtain a breakthrough of $CO_2$

$$\tilde{\omega}_1(\xi,\tau)=\tilde{\omega}_{11}(\xi,\tau)\theta(\xi_1-\xi)+\tilde{\omega}_{11}(\xi-\xi_1,\tau)\theta(\xi-\xi_1), \qquad (29)$$

where 1 on the left is the number of jumps in the diameter of the granules.

Similarly, for an inhomogeneous cartridge with two jumps in the diameter of the granules, we have

$$f_{3;0}(\tau)=\tilde{\omega}_1(\xi_2,\tau)e^{\alpha_3\tau}, \qquad f_{3;k+1}(\tau)=\alpha_3\int_0^{\tau} f_{3;k}(\tau)d\tau, \tag{30}$$

$$\tilde{\omega}_{23}(\xi,\tau)=e^{-\alpha_3(\xi+\tau)}\sum_{k=0}^{\infty}\frac{f_{3;k}(\tau)}{k!}(\alpha_3\xi)^k, \tag{31}$$

$$\tilde{\omega}_2(\xi,\tau)=\tilde{\omega}_1(\xi,\tau)\theta(\xi_2-\xi)+\tilde{\omega}_{23}(\xi-\xi_2,\tau)\theta(\xi-\xi_2), \tag{32}$$

which allows us to notice the general pattern ( $n=3,4,\ldots$ )

$$f_{n+1;0}(\tau)=\tilde{\omega}_{n-1}(\xi_n,\tau)e^{\alpha_{n+1}\tau}, \qquad f_{n+1;k+1}(\tau)=\alpha_{n+1}\int_0^{\tau} f_{n+1;k}(\tau)d\tau, \tag{33}$$

$$\tilde{\omega}_{n\,n+1}(\xi,\tau)=e^{-\alpha_{n+1}(\xi+\tau)}\sum_{k=0}^{\infty}\frac{f_{n+1;k}(\tau)}{k!}(\alpha_{n+1}\xi)^k, \tag{34}$$

$$\tilde{\omega}_n(\xi,\tau)=\tilde{\omega}_{n-1}(\xi,\tau)\theta(\xi_n-\xi)+\tilde{\omega}_{n\,n+1}(\xi-\xi_n,\tau)\theta(\xi-\xi_n). \tag{35}$$

The results of calculations performed according to formulas (33) – (35) in the environment of the MathCAD package are presented in graphical form in Figure 2.

Curves 1 and 3 are constructed according to formulas (8) and (17)-(19) ( $n=4$ ) for an open circuit. And curves 2 and 4 were constructed using an iterative procedure (the first approximation was found for a homogeneous cartridge and an inhomogeneous one with four jumps in the diameter of granules with a circular connection scheme, respectively).

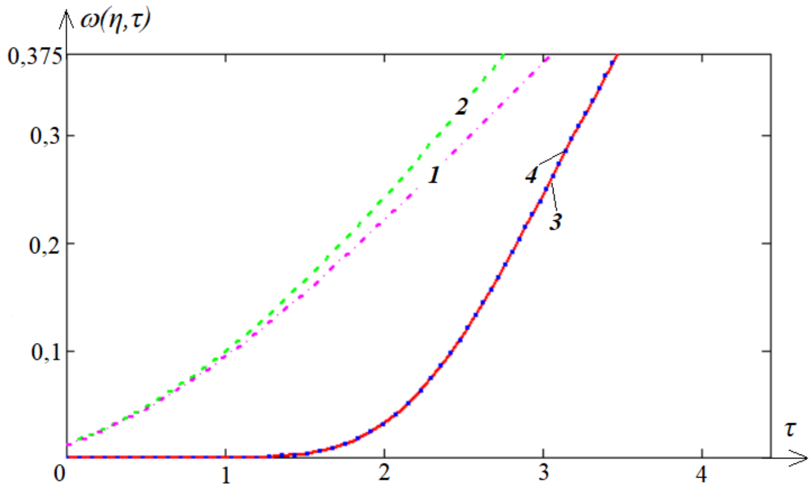



**Fig. 2. $CO_2$ slip through the regenerative cartridge uniformly equipped with open (1) and circular (2) connection schemes; with four jumps in the diameter of the granules in open (3) and circular (4) schemes**

It can be seen that curve 3 coincides with curve 4 (Fig. 2). This suggests that in a cartridge with four jumps in the diameter of the granules, the closedness of the airway part does not reduce the time of critical breakthrough as it does in a uniformly loaded cartridge (distance between curves 1, 2, increment 9.8%). The reason is that, due to the jumps in the diameter of the granules, the cartridge binds $CO_2$ molecules better and they practically do not return to inhalation, thereby not affecting the concentration of carbon dioxide in exhalation.

As a result, in an insulating apparatus with four jumps in the diameter of the granules (operating in a circular pattern), the increase in the time for the onset of a critical breakthrough (the distance between curves 2, 4 (Fig. 2)) will be 25.9%. This is almost twice the 13.7% increase in the open circuit (the distance between curves 1, 3 (Fig. 2)).

An increase of 25.9% practically coincides with the value found from the average contamination of the same cartridge with four jumps in the diameter of the granules connected in an open circuit (25.2%). This coincidence is not accidental and is a consequence of the law of conservation of carbon dioxide molecules. Indeed, the time of the onset of the critical breakthrough of $CO_2$ is determined by the number of molecules that have passed into the filter. And in a closed circuit it is equal to that produced as a result of human activity minus those absorbed by the cartridge. If the breakthrough increases more slowly, then the pollution grows faster. That is, the increase in protective action found since the critical break in the closed loop part of the duct will be equal to the increase in fixed carbon in the open loop.

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