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## **CO<sub>2</sub> binding by Baralyme in three different carrier gases**

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Lin M-J, Jaeger MJ. CO<sub>2</sub> binding by Baralyme in three different carrier gases. *Undersea Hyperbaric Med* 1994; 21(3):329-340.—The absorptive properties of Baralyme and Sodasorb for CO<sub>2</sub> in a container were studied by measuring the lifetime  $T_{0.5}$  of the unit, i.e., the time until the exit concentration of CO<sub>2</sub> reaches 0.5%. The container size, the inlet gas flow rate, and the inlet CO<sub>2</sub> concentration were varied. The experiments were repeated with either He, N<sub>2</sub>, or SF<sub>6</sub> as the inert gas to evaluate the effect of increased gas density due to hyperbaric conditions on scrubber performance. It was found that  $T_{0.5}$  is best described by an exponential function of the type  $b(t_t)^a$ , where  $t_t$  is the transit time of the gas through the container. The exponent  $a$  equals about 1.5 and varies relatively little. The constant  $b$ , however, is strongly dependent on inert gas density and on CO<sub>2</sub> concentration in the inlet gas; it is independent of container size and gas flow rate. In addition, the amount of absorber reacting up to time  $T_{0.5}$  was measured in all conditions. It is strongly dependent on CO<sub>2</sub> concentration; however, surprisingly it is nearly independent of inert gas properties. These results are compared with a mathematical model of scrubber behavior that is based on the chemical reaction rate of an imaginary absorber. The model neglects possible effects of CO<sub>2</sub> diffusion in the gas phase, of ash formation, and of heat produced by the reaction. Differences between our experimental data and the model are analyzed as a function of these effects. The results give some simple predictive equations for the lifetime and the amount of absorber reacting.

*CO<sub>2</sub> scrubber, CO<sub>2</sub> absorber, Baralyme, diving equipment*

The removal of CO<sub>2</sub> from gas mixtures in diving equipment, anesthesia machines, and, on a larger scale, in closed environments such as submarines is a routine procedure. One might expect, therefore, that the mechanisms involved in the working of these simple chemical absorbers (scrubbers) would be well understood. This is not the case. Many questions raised by this technology are still unanswered even though the basic chemistry is well known (1-4). This paper tries to add some theoretical and experimental information, especially with respect to the effect of the density of the carrier gas on the life of the absorber. Our main effort is toward finding some simplifying relationships that may aid in improving the design of practical equipment.

To analyze the factor we are most interested in, namely, the effect of the inert gas, we chose to compare our results with those of a mathematical model that is

attractive by its simplicity. It was derived by Houston et al. (5) and is based on a mathematical description of the chemical reaction only. The effects of diffusion in the gas phase and in the solid phase are neglected and so are effects of gas density. The temperature is assumed to be constant and the gas flow to be plug flow. The only variables are the volume of the container (which determines the amount of absorber), the chemical reaction rate, the inlet flow rate, and the inlet CO<sub>2</sub> concentration. This is summarized in the appendix, which also contains a glossary with a list of all variables, with the definition, symbol, and unit for each.

The theory defines important parameters, which are of great help in analyzing experimental data. Thus, the theory defines a time  $T$  needed for the reaction to come to an end because of consumption of the absorbent.  $T$  is defined by the ratio of absorbent quantity (in moles) divided by the rate of inflowing CO<sub>2</sub> (in moles per minute):

$$T = \frac{bdV_s}{M} \times \frac{V_M}{\dot{V}F_{I_{CO_2}}} \text{ (in min)} \quad (1)$$

where  $V_s$  is the volume of the scrubber,  $\dot{V}$  the gas flow rate, and  $F_{I_{CO_2}}$  the fraction of CO<sub>2</sub> at the inlet to the absorber; the other symbols represent physicochemical constants. The ratio  $V_s:\dot{V}$  signifies a time; if the gaseous space is expressed by multiplying  $V_s$  by the porosity  $\epsilon$ , the ratio  $t_{tr} = \epsilon V_s:\dot{V}$  becomes equal to transit or contact time. The above equation may then be rewritten as

$$T = \frac{t_{tr}}{F_{I_{CO_2}}} \times \frac{bdV_M}{\epsilon 60M} = \frac{t_{tr}}{F_{I_{CO_2}}} \times 9.32 \quad (2)$$

where  $t_{tr}$  is in seconds and  $T$  in minutes. For the values of the various physical constants, see the appendix.

The model predicts relationships between the independent variables,  $T$  and  $t_{tr}$ , and  $T_{0.5}$  which is the critically important, dependent variable.  $T_{0.5}$  is the lifetime of the scrubber; it is defined as the time when exit concentration reaches 0.5%. The definition is based on physiologic data which indicate that inspired gas containing more than 0.5% CO<sub>2</sub> may negatively affect performance and well being of the subjects. The model predicts that  $T_{0.5}$  is directly proportional to  $t_{tr}$  (appendix Eq. 5a). The slope of the linear relationships is determined by  $F_{I_{CO_2}}$ , the fraction of CO<sub>2</sub> at the inlet, and the reaction rate constant  $K$  of CO<sub>2</sub> with the absorber. This is illustrated in Fig. 1 where the slope of the  $T_{0.5}$  vs.  $t_{tr}$  relationship increases sharply when the inlet CO<sub>2</sub> fraction,  $F_{I_{CO_2}}$  is reduced. The slope also increases if the reaction rate  $K$  is higher. Comparison of the two panels in Fig. 1 indicates a strong interaction of the effects of  $F_{I_{CO_2}}$  and  $K$ : the effect of  $F_{I_{CO_2}}$  is less pronounced when  $K$  is large.

We propose to compare our experimental data with the model and to use the same  $T_{0.5}$  vs.  $t_{tr}$  relationship to plot them. Differences between model and experiment will be interpreted as being due to factors not included in the model such as diffusion and gas density.

## METHODS

We used a container 4.1 cm i.d. and 28 cm long which we filled to three different heights with absorber; this yields either 1.65, 1.98, or 2.64 mol of absorber. Usually

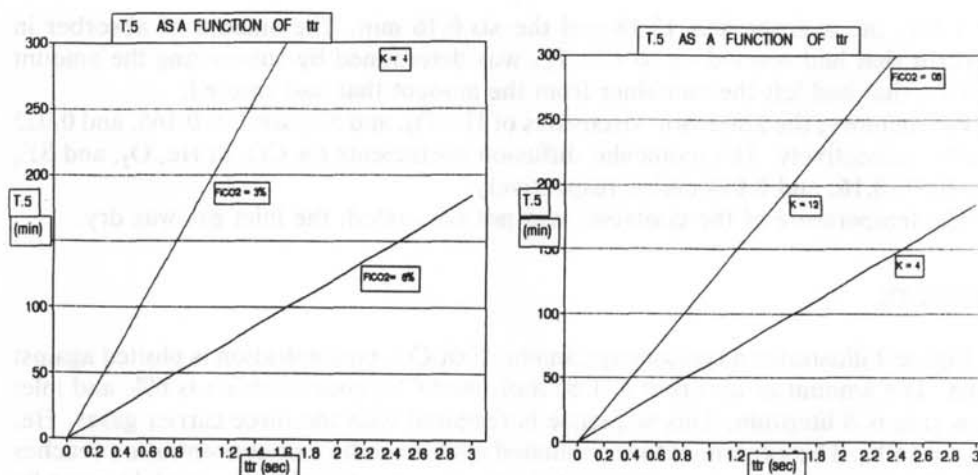


FIG. 1— $T_{0.5}$  vs.  $t_{tr}$  as predicted by the model. Constants are given in the appendix. *Left*, the effect of inlet CO<sub>2</sub> concentration (3 and 6%) if  $K$  is maintained constant; *right*,  $K$  is raised.

this absorber was Baralyme, but we also used Sodasorb. The composition of the two absorbers is shown in Table 1. The pellet diameter is 4–8 mesh. The canister is smaller than most commercial scrubbers, but appreciably larger than that of some previous authors (1, 3, 6).

The flow rate was set at either 2, 4, or 8 liters/min and the  $F_{I_{CO_2}}$  at either 0.03 or 0.06. Together with the variation of the amount of the absorber, this resulted in a range of  $T$  values between 77 and 985 min. The transit time  $t_{tr}$  varied between 0.5 and 3.2 s. The flow rate was varied stepwise in such a fashion as to keep inlet  $\dot{V}_{CO_2} = \dot{V} \times F_{I_{CO_2}}$  constant. This gave information on the possible effect of gas velocity while keeping the rate of inflow of CO<sub>2</sub> constant.

All experiments were repeated with either He, O<sub>2</sub>, or SF<sub>6</sub> as the carrier gas. They were conducted until  $F_{E_{CO_2}}$  reached 0.01. The value of  $T_{0.5}$  was then read, i.e., the time needed for  $F_{E_{CO_2}}$  to reach 0.005. The reproducibility of repeated experiments was good; one series of four experiments under the same conditions gave a variability

Table 1: CO<sub>2</sub> Absorbent Compositions and Densities

Absorbent	Composition, by weight, %	Bulk Density, g/ml	ABS Density, g/ml	Mesh	
Baralyme	Ca(OH) <sub>2</sub>	74	0.94	2.15	4–8
	Ba(OH) <sub>2</sub> ·8H <sub>2</sub> O	11			
	KOH	5			
	H <sub>2</sub> O	10			
Sodasorb	Ca(OH) <sub>2</sub>	80	0.745	2.49	4–8
	NaOH	5			
	KOH				
	Ba(OH) <sub>2</sub> ·8H <sub>2</sub> O				
	H <sub>2</sub> O				

of 1.3%; the average was 12.18 and the SD 0.16 min. The amount of absorber in percent that had reacted up to  $t = T_{0.5}$  was determined by subtracting the amount of  $\text{CO}_2$  that had left the container from the amount that had entered.

For memory, the kinematic viscosities of He,  $\text{O}_2$ , and  $\text{SF}_6$  are 1.3, 0.166, and  $0.022 \text{ cm}^2/\text{s}$ , respectively. The molecular diffusion coefficients for  $\text{CO}_2$  in He,  $\text{O}_2$ , and  $\text{SF}_6$  are 0.67, 0.16, and  $0.074 \text{ cm}^2/\text{s}$ , respectively.

The temperature of the container was not controlled; the inlet gas was dry.

## RESULTS

Figure 2 illustrates a typical experiment. Exit  $\text{CO}_2$  concentration is plotted against time. The amount of absorber is 1.65 mol, inlet  $\text{CO}_2$  concentration is 6%, and inlet flow rate is 8 liter/min. This sequence is repeated with the three carrier gases, He,  $\text{O}_2$ , and  $\text{SF}_6$ . The experiment is terminated each time the exit concentration reaches 1%. The shape of the curves obtained is convex as predicted by the model (appendix Eq. 3a). The values of  $T_{0.5}$  determined from the curves in Fig. 2 are 5.3, 7.4, and 11.5 min for the three gases, with the results in  $\text{SF}_6$  having the shortest life.

In the following three figures,  $T_{0.5}$  is plotted against  $t_{\text{tr}}$  to show the effects of inlet  $\text{CO}_2$  concentration (Fig. 3) and inert gas (Figs. 4 and 5). Note that all lines are curvilinear. The effect of type of inert gas is appreciable, with He resulting in a distinctly higher lifetime than either  $\text{O}_2$  or  $\text{SF}_6$ .

For each of the three inert gases used, we chose to run experiments at twice the gas flow but half the inlet  $\text{CO}_2$  concentration. This reduced the  $T_{0.5}$  drastically. These results are discussed in more detail in the discussion. Since all relationships of  $T_{0.5}$  vs.  $t_{\text{tr}}$  are found to be ailinear, we describe these relationships by the regression equation

$$T_{0.5} = b \times t_{\text{tr}}^a \quad (3)$$

where  $b$  and  $a$  are regression coefficients.

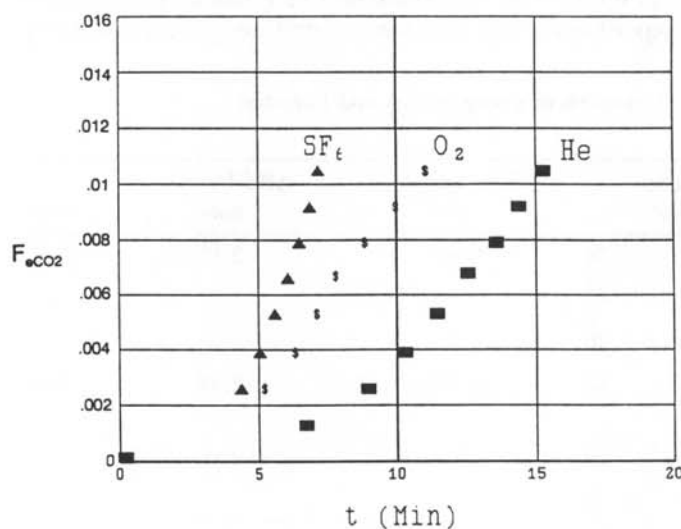


FIG. 2—Time course of exit  $\text{CO}_2$  concentration obtained experimentally in Baralyme with three different gases. Conditions are: 1.65 mol of absorber, gas flow rate 8,000 ml/min,  $F_{\text{I}\text{CO}_2} = 0.06$ .

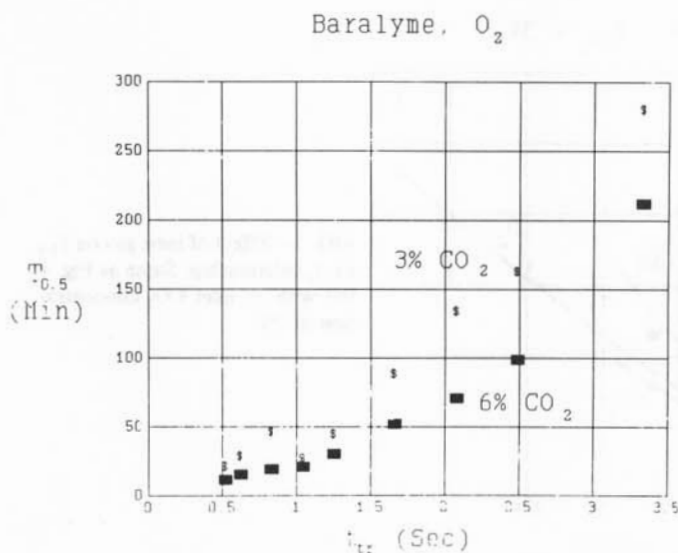


FIG. 3—Relationship between the life of the scrubber  $T_{0.5}$  and  $t_{tr}$ , the transit or contact time at two different inlet concentrations, Baralyme; inert gas: O<sub>2</sub>. Regression equations are listed in Table 2.

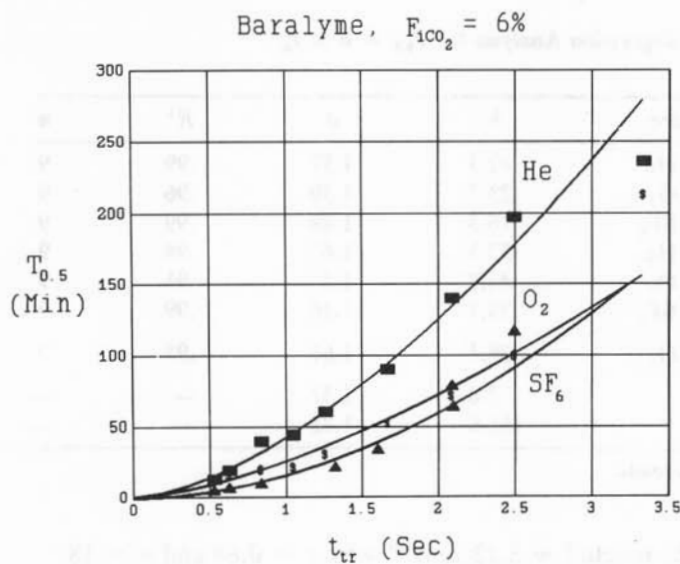


FIG. 4—Effect of inert gas on  $T_{0.5}$  vs.  $t_{tr}$  relationship. Baralyme, inlet CO<sub>2</sub> concentration 6%; inert gas: He, O<sub>2</sub>, or SF<sub>6</sub>. Regression equations are listed in Table 2.

The results of the statistical analysis are given in Table 2. The curvature of the relationships indicated by the exponent  $a$  seems to be fairly constant. The slope  $b$  of the relationships, however, varies greatly with CO<sub>2</sub> concentration and with type of gas. Table 2 also shows that Sodasorb provides for distinctly greater canister life than Baralyme.

The amount of absorbent in percent that has reacted when the exit CO<sub>2</sub> concentration reaches 0.5% is plotted in Figs. 6. It is seen that the data points are clustered along two curved lines, one for  $CI_{CO_2} = 3\%$  and the other for  $CI_{CO_2} = 6\%$ . Each line implies that there is a single relationship between  $T_{0.5}$  and percent of the absorbent that has reacted and that this relationship is independent of velocity, length, and gas properties. The two regression relationships are:

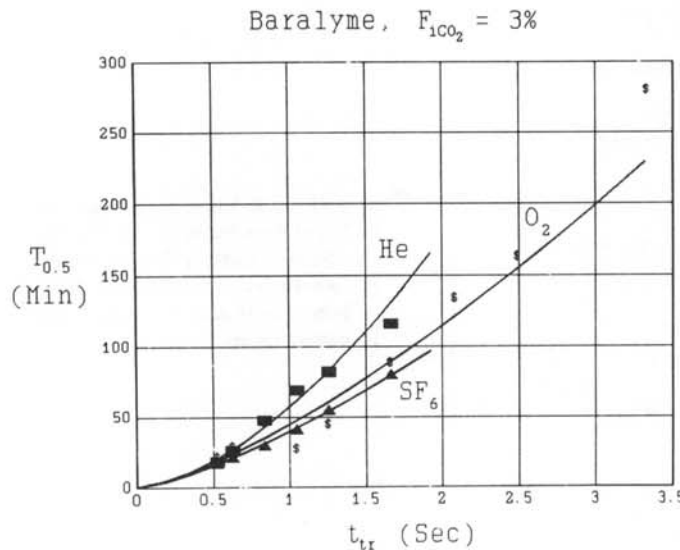


FIG. 5—Effect of inert gas on  $T_{0.5}$  vs.  $t_{tr}$  relationship. Same as Fig. 4 but with an inlet  $CO_2$  concentration of 3%.

Table 2: Regression Analysis for  $T_{0.5} = b \times t_{tr}^a$

Absorbent	Gas Mixture	$b$	$a$	$R^2$	$n$
Baralyme	6% $CO_2$ in He	42.3	1.57	.99	9
	6% $CO_2$ in $O_2$	25.7	1.50	.96	9
	6% $CO_2$ in $SF_6$	16.3	1.89	.99	9
	3% $CO_2$ in He	57.3	1.62	.98	9
	3% $CO_2$ in $O_2$	44.7	1.36	.91	9
	3% $CO_2$ in $SF_6$	39.7	1.36	.99	9
Sodasorb	6% $CO_2$ in $O_2$	38.1	1.61	.95	9
LiOH	4.4% $CO_2$	7.0	1.32	—	—
	1.1% $CO_2$	155.6	1.73	—	—

Note:  $T_{0.5}$  is in minutes;  $t_{tr}$  is in seconds.

For inspired  $CO_2 = 3\%$  : % reacted =  $3.12(T_{0.5})^{0.40}$  with  $r = 0.88$  and  $n = 18$ .

For inspired  $CO_2 = 6\%$  ; % reacted =  $3.26(T_{0.5})^{0.48}$  with  $r = 0.93$  and  $n = 27$ .

## DISCUSSION

The experimental data show consistently an alinear relationship between the life of the scrubber  $T_{0.5}$  and the transit time  $t_{tr}$  (Figs. 3–5). The mathematical model, however, predicts linearity (Fig. 1). The difference is almost certainly due to the assumptions at the basis of the model which neglect the possible effects of temperature, accumulating end products of the chemical reactions, diffusion, and gas density. We chose to express the curvilinear data with an exponential relationship largely for

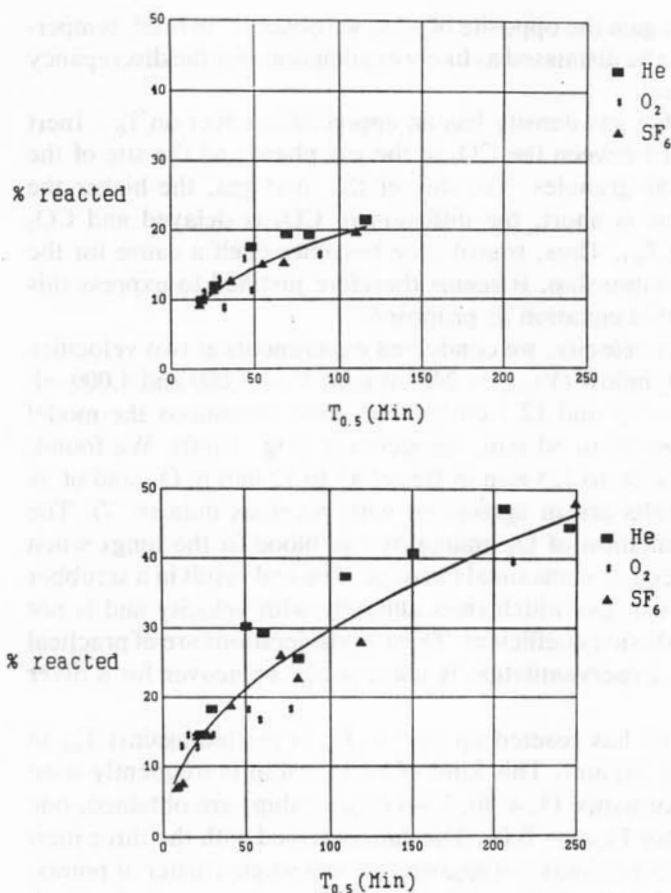


FIG. 6—Relationship between amount of absorbent that has reacted as a percent of the total amount available at the beginning is plotted against  $T_{0.5}$  for two different inlet CO<sub>2</sub> concentrations. Top, 3% and the regression yields  $3.12 \times (T_{0.5})^{0.4}$ ; bottom, 6% and the regression yields  $3.26 (T_{0.5})^{0.48}$ . Correlation coefficients are 0.95 and 0.9, respectively.

statistical reasons; it gives a series of excellent correlation coefficients (Table 2.). We found also theoretical support for this approach and discuss it later.

The theory points to the reaction rate constant  $K$  and to  $F_{I_{CO_2}}$  as to the factors that determine the slope of the  $T_{0.5}$  vs.  $t_{tr}$  relationship (Eq. 5a; Fig. 1). An increase of  $K$  leads to a steeper slope. Presumably,  $K$  increases with reaction temperature; thus, if temperature were to increase with increasing  $t_{tr}$ , one might expect to find a curvilinearity of the type seen in Figs. 3–5. However, temperature almost certainly declines with increasing  $t_{tr}$  because we raise the transit time by lowering the rate of inflowing gas. This reduces the rate of inflowing CO<sub>2</sub>, reduces the rate of chemical reactions, and probably reduces the temperature of the scrubber. Thus, one expects a curvilinearity which is concave to the X-axis rather than convex, as observed.

The end products of the chemical reaction, salts and water, are the second confounding factor to be considered. Figure 6 shows that the amount of end products increases with increasing value of  $t_{tr}$ . Since the end products accumulate on the outside of the absorber granules, they result in a barrier of increasing thickness between CO<sub>2</sub> in the gas phase and the absorber, and reduce scrubber life. Thus one expects the accumulation of end products to result in a  $T_{0.5}$  vs.  $t_{tr}$  relationship with

concavity toward the X-axis, again the opposite of what we observe. In brief, temperature and end products have to be dismissed as likely explanations for the discrepancy between model and experiment.

Figures 2, 4, and 5 show that gas density has an appreciable effect on  $T_{0.5}$ . Inert gas acts as a diffusion barrier between the  $\text{CO}_2$  in the gas phase and the site of the chemical reaction on or in the granules. The denser the inert gas, the higher the effect. When the contact time is short, the diffusion of  $\text{CO}_2$  is delayed and  $\text{CO}_2$  appears at the exit, reducing  $T_{0.5}$ . Thus, transit time becomes itself a cause for the alinearity of the  $T_{0.5}$  vs.  $t_{tr}$  relationship. It seems therefore justified to express this relationship with an exponential equation as proposed.

To pinpoint the effect of gas velocity, we conducted experiments at two velocities but with the same rate of  $\text{CO}_2$  inflow ( $\dot{V}_{\text{ICo}_2} = 240$  ml/min;  $\dot{V} = 8,000$  and  $4,000$  ml/min;  $t_{tr} = 0.5$  and  $1.0$  s;  $v = 25$  and  $12.5$  cm/s). For these conditions the model predicts a decline of  $T_{0.5}$  from 90 to 60 min, respectively (Fig. 1 *left*). We found, however, an increase of  $T_{0.5}$  of 56 to 125 min in He, of 45 to 72 min in  $\text{O}_2$ , and of 39 to 59 min in  $\text{SF}_6$ . These results are in agreement with previous data (6, 7). The mechanism is akin to the limitation of  $\text{O}_2$  uptake by the blood in the lungs when contact time is critically reduced as in maximal exercise. The end result in a scrubber is an increase of  $\text{CO}_2$  in the exit gas which rises alinearly with velocity and is not directly proportional to the diffusion coefficient. These considerations are of practical significance. They show that hyperventilation is not a useful maneuver for a diver using a scrubber.

The amount of absorber that has reacted up to  $t = T_{0.5}$  is plotted against  $T_{0.5}$  in Fig. 6 as percent of the initial amount. This kind of relationship is frequently used in the study of scrubber performance (3, 4, 6). Two relationships are obtained, one for  $\text{FI}_{\text{CO}_2} = 0.03$ , the second for  $\text{FI}_{\text{CO}_2} = 0.06$ . The data obtained with the three inert gases (He,  $\text{O}_2$ , and  $\text{SF}_6$ ) are, surprisingly, all aggregated on a single cluster of points; in this cluster one can still identify three somewhat distinct curves, one for each gas; however, the distinction is not nearly as noticeable as in Figs. 4 and 5, where the same data points form three different regression curves. This observation has a mathematical explanation.

It may be shown that the concave relationships seen in Fig. 6 are the mere mirror-images of the convex relationships in Figs. 4 and 5. Indeed, using Eqs. 2 and 7a one may derive algebraically that if

$$T_{0.5} = b \times t_{tr}^a \quad (3)$$

$$\% \text{ reacted} \approx \frac{T_{0.5}}{t_{tr}} \approx b^{1/a} \times (T_{0.5})^{1-1/a} \times \frac{\text{FI}_{\text{CO}_2}}{9.32} \quad (4)$$

It may be seen that the plotting of  $T_{0.5}/t_{tr}$  against the ordinate  $T_{0.5}$  diminishes the "separation" of the three lines in Figs. 4 and 5, which tend to merge into one "cluster" of points in Fig. 6.

There is disagreement as to the effect of diving depth on scrubber performance. Some papers (6–10) describe an effect but disagree on its magnitude; another paper (9) found no effect. These discrepancies are due, presumably, to methodologic differences; they are also because the standard method of evaluating the performance is



to compute the amount of absorber that has reacted as in Fig. 6. As has been discussed above, this index is not discriminative. Middleton (7), who used gases of different density and who also varied ambient pressure, found effects that interacted with the scrubber temperature. Such interactions are predicted by *Eq. 5a* and illustrated with Fig. 1 since the reaction rate constant  $K$  is dependent on temperature.

Depth affects performance through two potential mechanisms. It results in a decrease of  $F_{\text{CO}_2}$  and in an increase of inert gas density. The decrease of the CO<sub>2</sub> fraction has no effect on the chemical behavior of the scrubber since it affects both  $F_{\text{I}_{\text{CO}_2}}$  and  $F_{\text{E}_{\text{CO}_2}}$  in *Eq. 5a*; depth has no effect on  $t_{\text{tr}}$  either. Any possible effect is therefore due to a decrease of temperature and of  $K$  or to the decrease of CO<sub>2</sub> diffusivity because of an increase of inert gas density, or both. The kinetic gas theory predicts that the binary molecular diffusion coefficient is inversely related to pressure (11). This is mimicked in some experiments, including ours, by changing the molecular weight of the inert gas. Thus, for example, the diffusivity of CO<sub>2</sub> in SF<sub>6</sub> is 9 times lower than in He (12). This corresponds to a change of pressure of 9 atm or to a depth of approximately 300 ft. Note, however, that the effects of density is relatively small: we varied inert gas density by nearly 3,600% and observed a variation of  $T_{0.5}$  by only about 50% (Figs. 4 and 5).

The data presented in this paper, though theoretically involved, provide simple, useful guidelines for the design of the scrubber:

1. The life of a scrubber is longer when the inlet CO<sub>2</sub> concentration is high and gas flow rate is low (assuming the same inflow of CO<sub>2</sub>). In an example given earlier, a reduction of gas flow to half raised the life from 45 to 72 min with O<sub>2</sub> as inert gas. For He, the increase was from 56 to 126 min.
2. The life of a scrubber is appreciably longer in He than in a heavier gas. This ought to be helpful in the design of closed-circuit systems designed for high performance.
3. The contact time is critical for the design. This is implied in the relationship  $T_{0.5} = b(t_{\text{tr}})^a$ . Thus, an increased transit time built into a system by increased absorber size may be useful despite the increased weight.
4. The amount of CO<sub>2</sub> bound in percent of capacity is closely related to the  $T_{0.5}:T$  and  $T_{0.5}:t_{\text{tr}}$  ratios. This simple relationship is embodied in *Eqs. 7a* and 4, respectively. It is easy to show that the factor after the ln sign in *Eq. 7a* affects the percent reacted by only a few percent.

The above guidelines might be useful in designing an underwater closed circuit intended as a backup for emergencies. Assume an average scrubber volume of 2 liter and an expired CO<sub>2</sub> concentration of 4.5%. The minute volume is assumed to be 75 liter/min for this emergency situation.  $T$  for this system equals 133 min,  $t_{\text{tr}} = 0.64$  min,  $T_{0.5}$  is less than 20 min, and the amount of the absorber used when  $t = T_{0.5}$  is about 14%. If the canister is increased to 2.5 liter and the assumed exercise level is reduced so that the average minute volume is 65 liter/min, the life of the scrubber increases substantially, especially in He ( $T_{0.5} =$  about 45 min). The utilization of the absorber rises to 23%.

Several questions remain unanswered by our study. They include the effect of uneven distribution of the gas flow through the unit which is referred to as channeling. This effect reduces the life of the scrubber and increases the variability of results. It is presumably related to the rate of CO<sub>2</sub> inflow, to heat and water production, to

cooling, and to continuous vs. discontinuous use. These factors are interdependent in their effects and are also dependent on the geometry and size of the unit. Our definition of  $t_{tr} = \epsilon V_s / \dot{V}$  does not account for these factors. Cooling through heat loss from the surface of a unit may be quite satisfactory, and temperature therefore constant in units with a very small diameter (1 cm) used in some experiments. We prefer a unit that comes closer in size to commercial units.

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## APPENDIX

### List of symbols with definitions, units, and nominal numerical values

A	Canister cross section area (cm <sup>2</sup> ); in the setup: 13.2 cm <sup>2</sup>
F <sub>CO<sub>2</sub></sub>	Concentration of CO <sub>2</sub> (cm <sup>3</sup> /cm <sup>3</sup> )
F <sub>I<sub>CO<sub>2</sub></sub></sub>	Concentration of CO <sub>2</sub> at the entrance of scrubber (cm <sup>3</sup> /cm <sup>3</sup> ); either 0.03 or 0.06
F <sub>E<sub>CO<sub>2</sub></sub></sub>	Concentration of CO <sub>2</sub> at the exit of scrubber (cm <sup>3</sup> /cm <sup>3</sup> )
L	Scrubber length (cm); in the setup: 12.5, 15, or 20 cm
M	Molecular weight of absorbent (g/mol); 94.1 g/mol
R	Reaction rate of CO <sub>2</sub> with absorbent (nondimensional)
V <sub>s</sub>	Scrubber volume (cm <sup>3</sup> ); in the setup: 165, 198, or 264 cm <sup>3</sup>
V <sub>m</sub>	Volume of 1 mol of ideal gas (cm <sup>3</sup> /mol); 22,400 cm <sup>3</sup> /mol
$\dot{V}$	Inlet gas flow rate (cm <sup>3</sup> /min); 2,000, 4,000, 8,000 cm <sup>3</sup> /min
n <sub>0</sub>	Initial absorbent concentration (g/cm <sup>3</sup> ) = vs. × b.d
t	time (min)
v	Effective speed of flow of gas through absorbent = V/εA (cm/s)
z	Axial distance from the entrance (cm)
b.d	bulk density (g/cm <sup>3</sup> ); 0.94 g/cm <sup>3</sup>
ε	porosity; 0.4

### List of dimensionless quantities

ξ	Dimensionless distance = z/liter
τ	Dimensionless time = tvF <sub>I<sub>CO<sub>2</sub></sub></sub> /Ln <sub>0</sub>
γ	Dimensionless absorbent concentration = absorbent concentration (ξ, τ) in molar units/initial absorbent concentration in molar units
χ	= Dimensionless CO <sub>2</sub> concentration, $\chi(\xi, \tau) = F_{CO_2}(z, t)/F_{I_{CO_2}}$
K	Coefficient of reaction rate

### Mathematical model

- Isothermal incompressible plug flow
- Axial and radial dispersion are neglected
- Reaction rate is proportional to the concentration of CO<sub>2</sub> and of the absorbent and is expressed in the form,  $R(\chi, \gamma) = K\chi\gamma$
- CO<sub>2</sub> concentration χ has the following dependence on the absorbent concentration γ

$$\chi(\xi, \tau) = \frac{\gamma(\xi, \tau) - \gamma(0, 0)}{\gamma(0, \tau) - \gamma(0, 0)}$$

Houston et al. (5) derived the following solution for this equation

$$\chi(\xi, \tau) = \frac{e^{K(\tau-1)}}{1 - e^{-K}(1 - e^{K\tau})}$$

Using dimensional variables listed earlier and defining,  $T$  = molar amount of absorber/molar flow of CO<sub>2</sub>

$$T = \frac{V_s(\text{bd}) V_m}{M\dot{V}F_{\text{CO}_2}} = \frac{t_{\text{tr}}(\text{bd}) V_m}{\epsilon M F_{\text{CO}_2}} \quad (1a)$$

where

$$t_{\text{tr}} = \epsilon V_s / \dot{V} \quad (2a)$$

we obtain

$$\frac{F_{\text{CO}_2}(L, t)}{F_{\text{I}_{\text{CO}_2}}} = \frac{e^{K(\frac{t}{T}-1)}}{1 - e^{-K} + e^{K(\frac{t}{T}-1)}} \quad (3a)$$

From this we derive the reaction rate of CO<sub>2</sub> with the absorber as a function of time

$$\text{reaction rate} = \dot{V}F_{\text{I}_{\text{CO}_2}} \left( 1 - \frac{e^{K(\frac{t}{T}-1)}}{1 - e^{-K} + e^{K(\frac{t}{T}-1)}} \right) \quad (4a)$$

and by integration the time  $t = T_{0.5}$  needed for  $F_{\text{E}_{\text{CO}_2}}$  to reach 0.005

$$T_{0.5} = \left[ 1 + \frac{1}{K} \text{Ln} \frac{1 - e^{-K}}{(F_{\text{I}_{\text{CO}_2}}/F_{\text{E}_{\text{CO}_2}}) - 1} \right] \frac{t_{\text{tr}}}{F_{\text{I}_{\text{CO}_2}}} \left( \frac{223.8}{\epsilon 60} \right) \quad (5a)$$

or

$$T_{0.5} = \left[ 1 + \frac{1}{K} \text{Ln} \frac{1 - e^{-K}}{(F_{\text{I}_{\text{CO}_2}}/F_{\text{E}_{\text{CO}_2}}) - 1} \right] T \quad (6a)$$

and finally the amount of absorber in percent that has reacted at  $t = T_{0.5}$

$$\% \text{ reacted} = \left( \frac{T_{0.5}}{T} - \frac{1}{K} \text{Ln}[1 - e^{-K} + e^{K(\frac{T_{0.5}}{T}-1)}] \right) \times 100 \quad (7a)$$

Note that  $T$  in Eq. 7a is closely related to  $t_{\text{tr}}$  in Eq. 1a.

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