

TITLE: A mathematical computer simulation of bottled
oxygen-type respirators and human subjects.

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ABSTRACT

We developed a mathematical model of bottled oxygen type respirators and human subjects using a computer simulation to aid in the designing and testing of **self-contained** breathing apparatus (**SCBA**). Input variables to the human side of the model enable one to describe any human subject during changing work loads. The model iterates on a **breath-by-breath** basis as opposed to the classical iteration technique using increments of time much shorter than the period of a breath. This enables the model to run faster than real-time on a small laboratory computer. The model predicts and records inspired and expired O_2 , CO_2 and nitrogen (N_2) fractions at the mouth for each breath. Total CO_2 absorbed and O_2 produced by the respirator are also predicted and recorded. The entire model was validated by constant flow-rate experiments (Kyriazi, 1984) and data collected on human subjects performing National Institute for Occupational Safety and Health (**NIOSH**) respirator certification tests (**i.e.**, Man tests 2 and 4). A nitrogen buildup condition was simulated. It was found that by decreasing the initial respirator bag volume the problem could be eliminated. The model has potential uses as both an educational tool for the industrial **hygienist** and in the design and testing of new respirators.

INTRODUCTION

Over the past ten years, the Bureau of Mines has conducted research aimed at maximizing the opportunities of an individual miner surviving a mine disaster, either by escaping from the mine or by being rescued by a team sent into the mine from the surface. If a mine disaster occurs, the atmosphere can become oxygen (O_2) deficient or contaminated with toxic gases, making escape or rescue impossible without the aid of a self-contained breathing apparatus (SCBA) to provide a respirable atmosphere.

One design of a SCBA supplies O_2 of high purity from a bottle to meet the **wearer's** metabolic demands, while removing the carbon dioxide (CO_2) from the expired breath by means of a chemical **sorbent** or scrubber.

A model of an SCBA and its wearer was constructed. It consists of a group of computer programs, written in the FORTRAN language, which simulate the dynamic changes in respired gas characteristics during various test paradigms of interest. Several limitations exist within the **model's** present framework. The model does not take into account variations in temperature or pressure. It assumes that the gases within the human subject, respirator, and dead space compartments of the model are perfectly mixed, ideal gases at standard temperature (0 degrees C) and pressure (760 mmHg). **Futhermore** it considers all gases to be dry. These

assumptions were made since the mantest data, with which the model was validated, was corrected to STPD.

The Model

A diagram of a human and respirator simulation (Figure 1) shows the relationships between the various parts of the model. Several areas of the block diagram can be changed easily to accommodate different types of respirators, as well as the wide variety of possible human parameters. The model can be described as a 4-compartment system consisting of a human lung, human dead space, respirator bag and a respirator dead space. CO_2 scrubbing characteristics of the respirator are determined in part by a "shrinking pore" model for the dynamics of the LiOH reaction. The "shrinking pore" model reduces the inside diameter of the simulated scrubber, thereby reducing the CO_2 scrubbing capacity as the reaction progresses.

The physiological input parameters for this study were obtained from tests of human subjects working under the National Institute for Occupational Safety and Health (NIOSH), 30 CFR Part 11 H, work protocols (NIOSH, 1976).

These parameters consisted of: (a) $\dot{V}\text{O}_2$, the rate at which the body is consuming oxygen O_2 , (b) $\dot{V}\text{CO}_2$, the rate at which the body is producing carbon dioxide (CO_2); (c) F_b , the frequency at which the subject is breathing; (d) $\dot{V}_E$, the total volume of air expired in one minute; and (e) TIME, the length of time this level of work must be continued.

Different physiologic input parameters are specified in an

attempt to simulate the actual rescue or escape experience, (e.g., an underground mine disaster).

The desired characteristics of any respirator design are used as input parameters. Basic variables include (a) maximum bag volume, (b) volume of O_2 available, (c) dead space within the breathing hoses, and (d) type of CO_2 scrubber. The scrubber can be changed from a uni-directional flow type canister to a bi-directional flow model. Once the overall scrubber's characteristics have been determined (including diameter, length and weight of LiOH present in the bed of the canister) the characteristics of the shrinking pore model are set, based on the size of the granules.

Various characteristics of the simulated human subject are specified, including: (a) functional residual capacity of the lung, which is a measure of the volume of the lung following a normal expiration; (b) anatomic dead space, the region of the human respiratory tract in which no gas exchange takes place, made up of the mouth, trachea, and bronchi. Input variables to the human side of the model include (a) work rate protocol, (b) dead space within the human respiratory tract, (c) functional residual capacity of the lung, and (d) the option of beginning the test with either an inspiration or an expiration.

Obviously the REMOD simulator software system itself cannot run, climb a ladder or do any physical labor. Therefore exercise has been performed by human subjects and

the intensity levels recorded. Average energy expenditure levels for various types of work are available in the literature (Kamon, Bernard and Stein 1975; Bernard, Kamon, and Stein 1979)

Once the parameters of the respirator and the human subject are specified, the simulation can begin with the first inspiration. The first calculation the model makes is an estimation of the fractional concentration of the gases passing by the mouth (Eq. 1).

$$F_{I O_2} = \frac{V_{RD} \times F_{L O_2} + (V_T - V_{RD}) \times F_{R O_2} + V_{O_2 DEM}}{V_T} \quad (1)$$

where: $F_{I O_2}$ = fraction O_2 inspired

$F_{L O_2}$ = fraction O_2 in lung

$F_{R O_2}$ = fraction O_2 in respirator

V_T = tidal volume

V_{RD} = volume dead space in respirator

$V_{O_2 DEM}$ = volume O_2 produced upon demand

Next it determines new lung volumes based on the air in the lung. Since the model iterates on a breath-by-breath basis and only reports values on the the half minute, we ignored the fluctuation in fractional concentrations at the mouth due to unequal mixing within the lung and the respirator's breathing bag.

Two separate measurements of inspired CO_2 concentration are made and recorded during the inspiratory phase of the breathing cycle. The first measurement is the average CO_2 concentration taken over an entire breath ($F_I CO_2$). The second measurement is the concentration of CO_2 at the distal end of the respirator breathing hose. The average CO_2 concentration, measured at the mouth over

an entire breath (i.e., the first measurement) will be significantly higher than that of the second measurement due to the inclusion in the former of the unscrubbed volume of CO_2 in the respirator's dead space.

A major assumption of the model is that all of the human gas exchange occurs during the inspiratory phase of the breathing cycle (Deno and Sittig, 1984). This major simplification is necessary if the breath-by-breath time incremental system is to be implemented. This assumption introduces a negligible error since we require that the total gas exchange during the inspiratory phase of the model be consistent with values measured on human subjects over an entire breathing cycle during actual human subject tests.

Most bottled oxygen respirators are equipped with a demand valve providing pure O_2 to the user when the pressure in the breathing bag drops below a set point. This drop in pressure corresponds to an empty breathing bag. Our model works on the basis of volumes, hence the demand valve is activated when the inspired volume exceeds the volume of gas within the breathing bag.

When the inspiratory phase is complete, the model begins the calculations for the expiratory phase. During sub-maximal work the volume of CO_2 produced is less than the volume of O_2 consumed. This means the volume of the human lung would continually decrease if both the inspired and expired tidal volumes were equal. On the other hand, at

maximal work loads in an anaerobic condition, the lung volume would increase due to the respiratory exchange ratio. Both of these conditions must be accounted for if the model's total gas volume is to stay constant throughout the changing work loads. The respiratory exchange ratio of the human subject is used to calculate the change in the expired volume as compared to the inspired tidal volume. This is done by modifying the expired tidal volume (2) by the difference between the oxygen consumption rate and the carbon dioxide elimination rate divided by the frequency of breathing.

$$V_{EXP} = V_T - \frac{(\dot{V}O_2 - \dot{V}CO_2)}{F_b} \quad (2)$$

where V_{EXP} = ~~is~~ expired tidal volume

V_T = & inspired tidal volume

$\dot{V}O_2$ = ~~is~~ oxygen consumption rate

$\dot{V}CO_2$ = ~~is~~ carbon dioxide elimination rate

F_b = ~~is~~ frequency of breathing

After the modification of expired tidal volume has been taken into consideration, the simulation determines the fraction of gases passing by the mouth. After the gas passes the mouth it enters the CO₂ scrubbing unit, which is represented by a shrinking pore model. The simulation calculates the concentration of CO₂ coming out of the LiOH

bed. It also calculates and records the scrubbing efficiency and total moles scrubbed.

Finally, the simulation determines the new volume of gas in the breathing bag, which is due to the influx (expiration) of gas from the human. Most respirator breathing bags are equipped with a relief valve to prevent the bag from over filling. This model incorporates this feature. It compares the new bag volume to the maximum bag volume, which is an input variable, and then finds the volume that needs to be vented.

The simulation increments on a **breath-by-breath** basis sending data to an averaging routine **after** every breath, from which half minute averages of an integral number of breaths are calculated and written to an output file, as well as being presented on the CRT screen. This output file contains the work rate; all of the human breathing characteristics; the inspired and expired gas fractions of O_2 , CO_2 , N_2 ; and the total amount (volume) of O_2 produced and CO_2 consumed by the respirator. The simulation also includes in its half minute reports the amount of O_2 received via the demand valve, the amount of gas vented and the scrubbing efficiency of the canister.

When the simulation has completed one entire breath, the protocol must be checked to determine whether a new work rate is required. This is done because the NIOSH human subject test protocols consist of a variety of work tasks which can

change every minute. If it **is**, the model reads in a new set of data and continues to breathe. If a new work load is not **required**, the model goes to the next phase of a breath and continues until the total time of the test is exceeded or until it is determined that the respirator has failed the test for any reason set forth in the NIOSH rules and **regulations**.

The CO₂ Scrubbing Properties of the Model

An important part of the REMOD simulation software system is the shrinking pore model used to represent the CO₂ scrubbing properties of the CO₂ absorbent canister within the respirator (Ramachandran and Smith, 1978; Chrostowski and Georgakis, 1978). This pore model simulates the scrubbing action of the lithium hydroxide (LiOH) in the **respirator's** absorbing canister.

"The absorption of CO₂ by LiOH is apparently a diffusion controlled **process**" (Boryta and Maas, 1982). With this in mind we decided to implement a kinetic reaction model based entirely on diffusion per the **aforementioned** papers which describe models of this type. A simplified version of these models was **necessarilly** implemented since: 1. The effect of chemical kinetics considered in previous papers are less important than the dynamics (dimensions) of bed configuration (Boryta and Maas, 1982). 2. The physical properties required of the reactant and the product are not all known. This problem was faced by the other authors when trying to validate their models. 3. The methods for solving

the differential equations involved are complex and time consuming. One of the main goals of the model was to have it run faster than real-time on a small computer. The models described in the published papers could not be solved within this time constraint. 4. Representing the functional characteristics of the CO_2 scrubber was more important to the overall study than requiring that the scrubber characteristics be determined from the most rigorous absorption models.

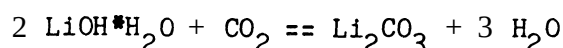
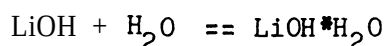
The overall chemical bed is divided into ten regions of equal volume representing the actual scrubbing bed within the respirator. The regions are divided along the axis of flow through the bed, with each region's pores being independent of the other nine regions of the bed. Each region contains a large number of "small" pores assumed to be homogeneously distributed (Figure 2). This allows plotting of the pore radius as a function of bed position. Also, the concentration of the outlet gas from each layer, or region, of the bed can be plotted, detailing the exact concentration profile within the scrubber.

The CO_2 absorption process within the CO_2 scrubbing canister can be thought of as a black box with two inputs (i.e., residence time (T_{RES}) and partial pressure of CO_2 for the j th region, ($P_j \text{CO}_2$) and one output ($P_o \text{CO}_2$). Ten state variables represent the pore radius (r_j , $j = 1, 2, \dots, 10$) of each individual layer within the canister. During each expiration, T_{RES} is calculated for all ten

regions, while $P_j\text{CO}_2$ and r_j are calculated for each region in sequence.

The residence time of the gas within each layer of the scrubbing canister is constant within each breath, but variable over the duration of the entire test, based on the ventilation rate ($\dot{V}_E$) of the human and the free air space within the chemical canister. The residence time is then calculated to be the time it takes for the gas to pass through the canister, assuming no change in pressure, during the expiration phase of a breath (assuming a 50% duty cycle).

Initially, all of the pores (i.e., r_j , where $j = 1, 2, \dots, 10$) are of the same radius. As the reaction progresses, each layer's pore radius shrinks based upon the change in molar volume of the reactant (LiOH 16.75 ml/mole) as it proceeds to the product stage (Li_2CO_3 35.7 ml/mole). It is known how many moles of CO_2 enter the region and the number exiting and therefore the number of moles of CO_2 absorbed. The number of moles of Li_2CO_3 formed is based on the stoichiometric relation:



Pore radius was then reduced as the reaction product accumulated. A weakness in our model is that the quantity of the intermediate product, $\text{LiOH} \cdot \text{H}_2\text{O}$ is not predicted; therefore, we used the theoretical value of 1:2, exclusively.

Model Validation

The model was validated by comparing model predictions to SCBA experimental measurement data (Kyriazi, 1984). Excellent agreement between measurements and predictions were achieved. Several explanations exist for the extreme similarity in data sets. Kyriazi used a metabolic breathing machine in place of a human subject for his tests (Kloos and Lamonica, 1966). This eliminated the problem of human subject variability so prevalent in the other human subject tests. Kyriazi also ran his tests at a low percentage of $\dot{V}O_2$. The model's two free constants were initially chosen based on data simulating low metabolic workloads. The data presented was the average of several trials. He presented the standard deviations (e.g., breakthrough time = 73 min $\pm$ 6 min) showing that even if the human subject variability is removed there still remains a significant amount of variability between supposedly identical respirator units.

Predictions of the model were next compared to experimental data gathered from human subjects during NIOSH Mantests 2 and 4. The graph of the inspired O_2 fraction (Figure 3) during mantest 4 agrees quite closely with the data from the human subjects. This is not surprising since there are fewer variables involved in the determination of the O_2 fraction both within the respirator and the simulation.

The graph showing the CO_2 fraction at the mouth (Figure 4) during mantest 2 shows less agreement with the human data. Although only one set of human data is plotted, several identical respirator units were run using the same NIOSH protocol. The variability of the inspired CO_2 concentration during each segment of the test was quite wide. There are many reasons for this variability. Differences in CO_2 production of the various human subjects caused by different fitness levels, weight, and efficiency in performing the work. Variability in the time and method of obtaining the gas samples during each work load. Small differences in the amount and packing of the LiOH in the absorbing canister. Slight changes in the feed rate of the constant supply of O_2 . Other miscellaneous changes in the basic operation of the respirator.

An important insight into the operation of respirators to come out of this simulation was the extreme sensitivity of the model, and hence the respirator, to small changes in the various characteristics of the respirator unit. During the evaluation of the CO_2 scrubbing portion of the model, for example, a one percent change in absorption capacity of the LiOH could mean a five to ten minute change in the break through time of the absorbent bed (i.e., the time for the CO_2 concentration in the inspired gas to reach 0.5 %).

The model was next used to simulate the effect of a method of correcting **or**, better yet, eliminating the nitrogen build-up problem. This **problem** occurs **when**, through an improper donning procedure, a large volume of nitrogen is introduced into the bag. Then the wearer begins to work at a $\dot{V}O_2$ which is above that of the constant O_2 bias flow **rate**. The result of these actions is that the O_2 concentration within the breathing bag can drop to dangerously **low** levels. A solution to this problem was found to consist of ridding the bag of excess gas by squeezing it immediately **after** donning the unit. This would activate the relief valve and cause the O_2 demand valve to be activated on the next inspiration which rapidly increases the O_2 concentration within the bag. This action, although seemingly costly in terms of O_2 waste, is not since this procedure would be used at a time when the O_2 concentration within the bag is low, hence the gas dumped is largely N_2 . Proper instruction in the donning procedure, coupled with this technique of ridding the system of excess nitrogen, should help to solve the nitrogen build-up problem.

The model was next used to show the importance of various physiological factors on respirator performance. The graph (Figure 5) shows the importance of the functional residual capacity (FRC) of the lung in determining inspired CO_2 levels helping to explain the problems involved with testing respirators on human subjects. The inter-subject variability is high enough to cause identical respirators to

fall the same test. Deno and reimers have addressed this problem and a solution is now available (1984). With the automated breathing, metabolic simulator (ABMS) the problem of variability in FRC of the subject has been eliminated (Deno, 1984).

Uses of the Model

A number of possible uses for the model exist within the research community as well as the respirator manufacturing industry. The simulation runs an order of magnitude faster than real time allowing one to make and see the effects of various design changes easily and quickly. This feature would be of great use early in the design process. For example: 1. One could change the amount of LiOH in the absorbent canister and find the corresponding change in breakthrough time of the CO₂. 2. The importance of breathing hose length and diameter in relation to inspired CO₂ concentration could be investigated by varying the dead space of the respirator. 3. The variability of human subject data could be quantified by inputting different human subject parameters with the same respirator characteristics and looking at the differences in the model's output (Sittig, 1984).

Another possible use of the model lies in its instructional value to the industrial hygiene professional. The affects of an improper donning procedure can be quickly and easily understood as one watches the various inspired and

expired gas fractions on the computer monitor. Also, the ability to "test" a new, or modified, respirator design by a computer simulation rather than by human **subject** may offer NIOSH a new tool with which to evaluate equipment submitted for certification. With a few small modifications in the model, **open-circuit** breathing apparatus designs could be simulated. Problems in the representation of a different air purifying system (**i.e.**, not LiOH) severely limit the **model's** use in the simulation of air purifying breathing apparatus design.

Acknowledgments

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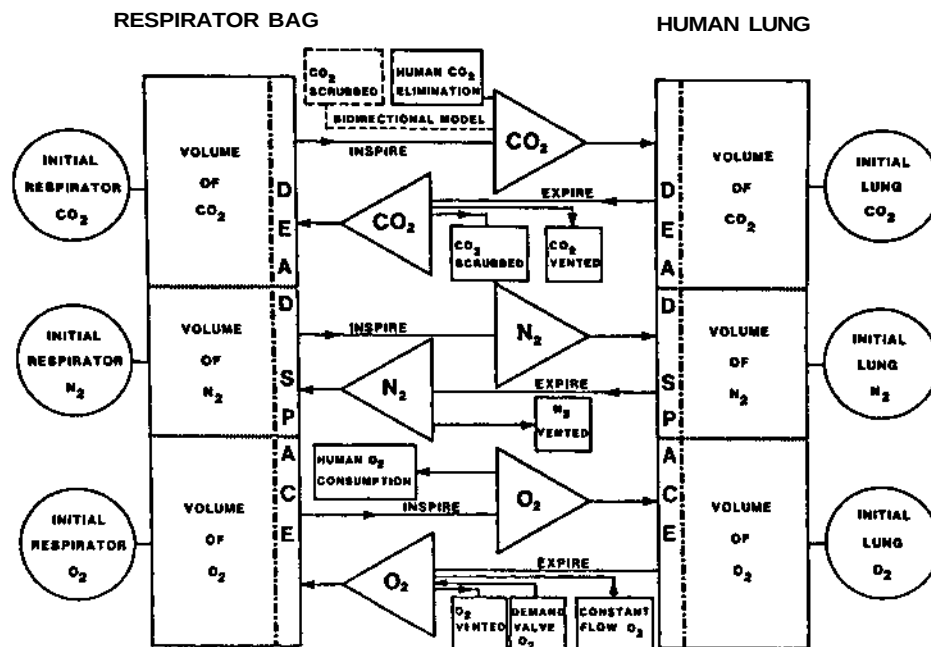


Figure 1. Block diagram of the respirator and human subject computer simulation

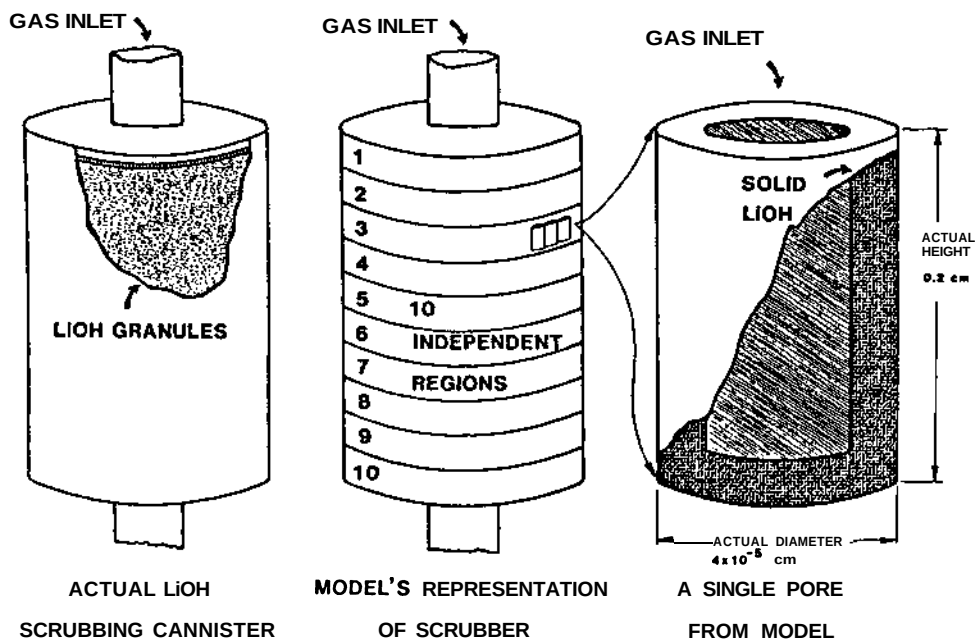


Figure 2. Diagram showing progression from actual respirator CO₂ scrubber to a single pore within the CO₂ scrubbing routine

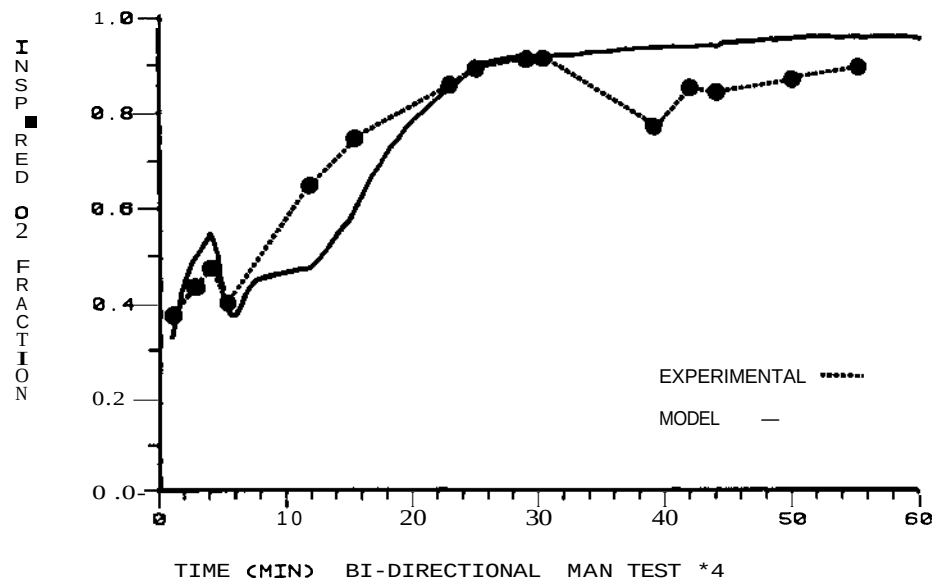


Figure 3. Inspired O₂ fraction at the mouth during NIOSH mantest 4 using a bi-directional flow respirator

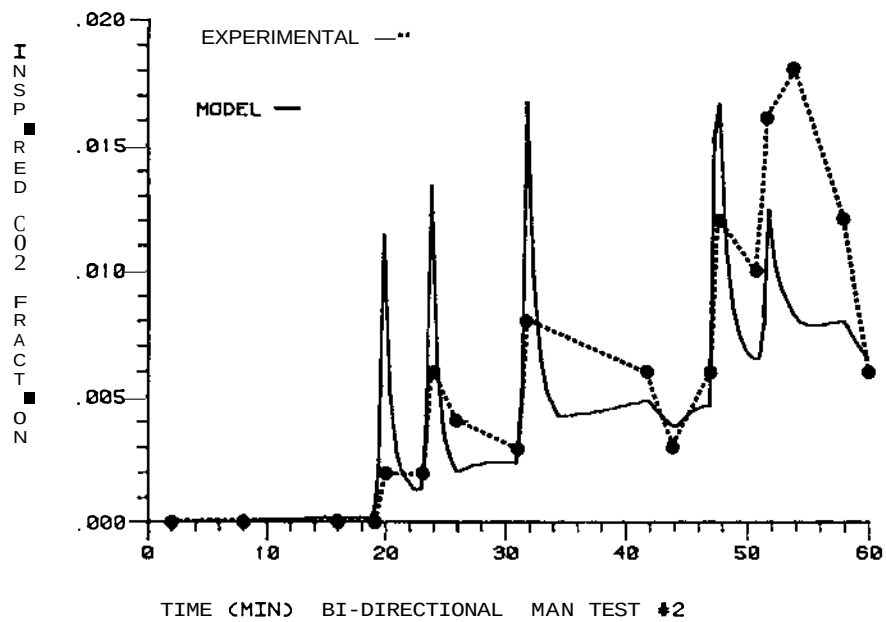


Figure 4. Inspired CO₂ fraction at the mouth during NIOSH mantest 2 using a bi-directional flow respirator

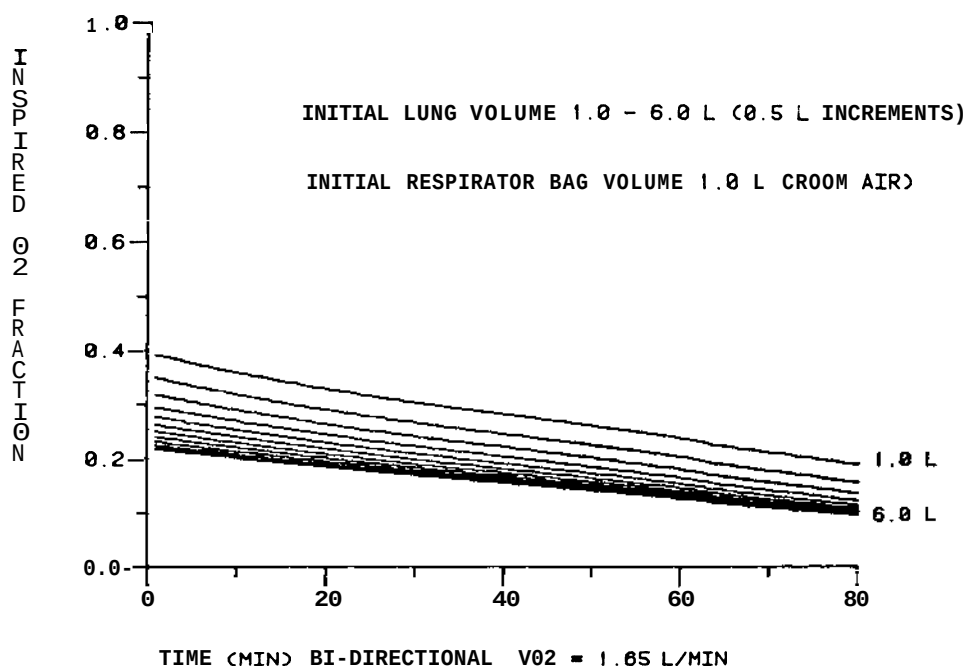


Figure 5. Responses of a bi-directional flow respirator, measured as inspired O₂ fraction, to various functional residual capacities (V_{O₂} = 1.65 l/min)