

SIMULATION OF GAS DYNAMICS IN A SUBJECT BREATHING VIA SELF-CONTAINED SELF-RESCUE APPARATUS

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Abstract. Self-contained self-rescue (SCSR) breathing devices are the only option for providing breathable air if hazardous components cannot be removed from external air after underground accidents. In this study, we developed a mathematical model of human breathing with an SCSR apparatus. The model describes the gas-content dynamics in the three system compartments: the lungs, body tissues and a SCSR apparatus. The results of simulations agreed well with experimental data obtained from a volunteer breathing through the apparatus.

Key words: alveolar gas exchange; mathematical modeling; self-contained breathing apparatus

1. INTRODUCTION

In industrial disasters such as underground accidents, ambient air can contain highly dangerous components, including carbon monoxide, and become irrespirable. In [1] the authors propose that facing a chemical, biological, radiological and nuclear incident, decontamination is a key element in safeguarding individuals and property. Decontamination is impossible in many underground incidents when safeguarding individuals could be obtained only with breathing apparatus. There are different techniques for providing safe respiration in such hazardous environments, including filtering half-masks, filtering full-face masks, and self-contained breathing apparatus. As a self-contained breathing apparatus does not use external air for respiration, it is the only suitable breathing apparatus when hazardous components cannot be removed from the surrounding external air.

There are three types of self-contained breathing apparatus: breathing apparatus with air- or oxygen-filled balloons and closed-circuit apparatus with chemically bound oxygen such as *self-contained self-rescue* (SCSR) devices without gas-filled balloons [2, 3]. Hence, prediction of the gas content in the inspired or expired air and blood of a subject breathing with SCSR device is a complicated problem in which simulations can be utilized.

Considerable information about respiratory gas dynamics during respiration through a breathing apparatus can be obtained by simulating breathing with an

SCSR device instead of performing actual experiments with human subjects. Such an application of a simulation approach with predictive model, based on the analytical solution of a system using differential equations, can be beneficial for designing self-contained breathing apparatus with chemically bound O₂ [4]. Bryant and Mensch developed a mathematical model of the flow across a flow resistance [5]. Simulations were conducted to predict the inward leakage into the facepiece of the breathing apparatus at high work rates, when the self-contained breathing apparatus may be overbreathed, *i.e.*, when the user requires more air than can be supplied.

Few studies have been devoted to simulation of chemical and physical processes in a self-contained breathing apparatus, but sufficient attention has not been paid to the physiology of human respiration [6–7].

The human respiration system reacts to the altered gas mixture while breathing with an SCSR device. Alkali metal superoxide-based (KO₂, NaO₂) regeneration products contain chemically bound O₂ liberated by a heat-producing reaction, accompanied by the proportional absorption of CO₂ and the water vapor present in the expired air. The user then inhales air with a high O₂ concentration, variable water vapor concentration, and slightly increased CO₂ concentration.

In 2001, Magosso and Ursino studied the effects of changes in the arterial CO₂ tension on the cardiovascular system through a mathematical model, with the important implication that is useful for the analysis and rational interpretation of physiological human respiration data [8]. The model includes differential equations describing the chemoreceptor afferent pathways, efferent sympathetic activity, central nervous system response.

The described models could be beneficial for the development of SCSR devices and their usage procedures in emergencies. After obtaining the SCSR parameters during breathing by performing a few real experiments, mathematical simulations can reduce the number of replications with human subjects. The model can be used to obtain the breathing gas dynamics (O₂, CO₂) and expected lifetime of the SCSR in a specific replication using simulation data instead of actual experiments with human test subjects.

2. METHODS

The mathematical model describes gas exchange in the human cardiorespiratory system and an SCSR device. The model adopts the common approach generally applicable for simulating mass exchange processes in living systems, which are treated as lumped parameter systems, and is based on the mathematical model of the human ventilation response to hypoxic and hypercapnic gas mixture during rebreathing tests [9].

2.1. MODEL COMPARTMENTS AND BASIC EQUATIONS

In this study, the human body was divided into two compartments: the lungs and tissues [10]. The model includes an SCSR breathing circuit (consisting of a bag, pipes and a regeneration cartridge) as the third compartment. The mass balance equations for each compartment and for the gases in question are as follows:

$$\frac{d}{dt}(M_{ji}) = \sum_{j,i} J_{ji}, \quad (1)$$

where $j = T, L$, and S represent the body tissue, lung, and breathing circuit (SCSR device) compartments, respectively; $i = 1, 2, 3$ represent O_2 , CO_2 , and a mixture of other gases (nitrogen (N_2) and others) that do not participate in the metabolic and chemical reactions, respectively; t is the time; M_{ji} is the mass of gas i in compartment j ; J_{ji} is the mass flow of gas i in compartment j from all other compartments and the environment, as well as the production or consumption of gas i in compartment j .

Thus, this model is described by a system of following nine mass balance equations.

Tissue compartment:

$$\frac{d}{dt}(M_{Ti}) = [C_{ai}(t-t_1) - C_{vi}(t+t_2)] \times Q + J_i, \quad i = 1, 2, 3 \quad (2)$$

Lung compartment:

$$\frac{d}{dt}(M_{Li}) = [F_{Li} \times V'_{AI} - F_{Ai} \times V'_{AE}] - [C_{ai} - C_{vi}] \times Q, \quad i = 1, 2, 3, \quad (3)$$

where C_{vi} and C_{ai} are the gas i contents in venous and arterial blood, respectively; F_{Ai} and F_{Li} are the gas i fractions in expired or inspired alveolar air (ratio of the gas i molecules to the total number of gas molecules); Q is the blood flow in the lungs and tissues; V'_{AI} and V'_{AE} are the alveolar inspiratory and expiratory ventilation, respectively; J_i is the gas i production or consumption rate in the tissue compartment; t_1 is the lung-to-tissue time delay, *i.e.*, duration for blood flow from the lung to tissue compartment; t_2 is the tissue-to-lung delay. When the O_2 consumption and CO_2 production in the lung tissue are much lower than those in the body tissues, Equation 3 neglects O_2 consumption and CO_2 production, by the lung compartment itself.

The governing equations for the pressure and gas fractions are as follows:

$$P = P_B - P_{\text{H}_2\text{O}}, \quad (4)$$

$$P_{ki} = P \times F_{ki}, \quad k = A, I, \quad i = 1, 2, 3 \quad (5)$$

$$\sum_{k,i} F_{ki} = 1, \quad i = 1, 2, 3; \quad k = A, I, \quad (6)$$

where P_B is the total gas pressure; P is the barometric pressure of dry gas; P_{ki} are the O_2 , CO_2 , and N_2 partial pressures in expired or inspired alveolar air (in the lung and SCSR compartments); and $P_{\text{H}_2\text{O}} = 47$ mmHg is the saturated water vapor pressure at the body temperature of 37°C . All of the other gases, except O_2 and CO_2 , are excluded from the metabolic and chemical reactions; hence $J_3 = 0$ and $R_3 = 0$. The fractions of N_2 and all of the other gases in the expired and inspired alveolar air can be completely determined using Equations 1–6 and the governing equations for the breathing circuit (SCSR device):

$$\frac{d}{dt}(M_{Si}) = F_{Ai} \times V'_{AE} - F_{Ii} \times V'_{Ai} + R_i + \frac{\Delta M_i}{\Delta t}, \quad (7)$$

where R_i is the O_2 emission and CO_2 absorption by the reagent as a function of time, which depends upon the regenerating agent properties, and ΔM_i is the amount of gas i discharged in a single valve actuation, which includes valve opening, gas discharge and valve closing. The single valve actuation duration was one discrete step (Δt) in the simulation.

The discharge mechanism in the model is as follows. Gas gradually accumulates within the SCSR bag due to the metabolic reactions in the human organism and the reagent heat-generation reaction. In the body compartment, there is metabolic O_2 consumption and CO_2 emission, while the regenerative cartridge releases O_2 and absorbs CO_2 proportionally; N_2 and the other gases are not involved in any reactions.

The total volume of the gas-exchange space, excluding the dissolved gas in the blood and tissues, consists of the alveolar volume of the lungs, physiological respiratory dead space and SCSR bag, pipes, cassette containing the regenerative cartridge, and equals 8 L. The SCSR bag was completely deflated at the beginning of the simulation, breathing commenced from resting expiration. Further, the volume of SCSR bag and the tidal alveolar volume changed due to inspiration and expiration, but the pressure in SCSR device was assumed to be 760 mmHg until the additional gas accumulated in the SCSR bag due to chemical and metabolic

reactions. Moreover, there was some gas expansion because the gas heating in the SCSR device and inspired volume steadily increased due to chemoreflex. The gas in the SCSR device was treated as a multicomponent gas mixture system. All of the gases except water vapor were assumed to behave ideally with overall pressure (P) defined by a constitutive equation of state corresponding to the ideal gas law, until the valve opened due to the pressure increase. The valve opening, gas discharge and valve closing duration was one discrete step (Δt) in the simulation. The pressure relief valve opened immediately after the pressure within the system reached 768 mmHg, and the excess gas mixture (ΔM) was removed. ΔM was estimated as the mean value obtained for 10 valve actuations by measuring the gas flow through the valve during the experiment and was approximately 0.6 L.

After the valve closed, the system pressure was assumed to be equal to the environmental air pressure, 760 mmHg. Excess gas discharge occurred immediately; however, the gas temperature in the SCSR before and after such discharge remained constant. Until valve actuation, the system was considered closed, and the gas dynamics in the system was described by the ideal gas law. Between the opening and closing of the valve, the system was open; hence, ΔM could only be obtained experimentally.

2.2. SPECIFIC EQUATIONS OF THE HUMAN-BODY COMPARTMENTS

The total gas content in the tissues and the total gas dissolved in the blood are described by the following equations [10]:

$$M_{Li} = F_{ai} \times (V_{alv} + V_{LT} \times \alpha_{Li} + V_{Lbl} \times \alpha_{bli}) + V_{Lbl} \times N_i \times S_{ai}^{Hb}, \quad i = 1, 2, \quad (8)$$

$$M_{Ti} = P_{vi} \times (V_{CT} \times \beta_{Ti} + V_{Cbl} \times \beta_{bli}) + V_{Cbl} \times N_i \times S_{vi}^{Hb}, \quad i = 1, 2, \quad (9)$$

$$V_{alv} = V_{0alv} + V_{talv}, \quad (10)$$

where V_{0alv} is the end tidal alveolar volume of the subject; V_{talv} is the tidal alveolar volume; V_{LT} and V_{CT} are the volumes of the pulmonary and body tissues of the subject, respectively; α_{Li} is the solubility of the gas i in the pulmonary tissues of the subject; β_{Ti} is the solubility of the gas i in the body tissues of the subject; V_{Lbl} and V_{Cbl} are the blood volumes in the lungs and body of the subject, respectively; α_{bli} is the solubility of the gas i in the blood of the lung compartment; β_{bli} is the solubility of the gas i in tissue compartment; N_i is the relative hemoglobin affinity to O_2 and CO_2 ; S_{ai}^{Hb} and S_{vi}^{Hb} are the hemoglobin saturation with O_2 and CO_2 in arterial and venous blood, respectively.

The gas transport properties of blood were defined using the equations developed by Hill that describe the Bohr and Haldane effects [11].

The pulmonary mechanics is represented as an inspired volume (V_t) function of time:

$$V_t = V_T \times |\sin(\omega \times t)|, \quad (11)$$

$$V_T = V_{talv} + V_{DC}, \quad (12)$$

$$\omega = \frac{2 \times \pi}{T_{BC}}, \quad (13)$$

where V_T is the tidal volume including the tidal alveolar volume V_{talv} and the physiological dead space V_{DC} ; ω is the cyclic respiration rate; and T_{BC} is the duration of two breathing cycles.

Ventilation is controlled by both peripheral and central chemoreflexes. The chemoreflexes and the relationship between the ventilation, tidal volume, and respiratory rate on one side and the CO_2 and O_2 partial pressures in the arterial blood on the other side, were simulated by imposing the perspective of Magosso and Ursino [8].

2.3. SPECIFIC EQUATIONS OF THE SCSR MODEL

The CO_2 consumption by the reagent is described as follows:

$$R_{\text{CO}_2} = k_{\text{CO}_2} \times F_{\text{ACO}_2} \times V'_{\text{AE}}. \quad (14)$$

We suggest that the reagent absorbs a fixed portion of CO_2 expired into the SCSR device, where the CO_2 absorption factor is given by:

$$k_{\text{CO}_2} = \frac{F_{\text{ET}}\text{CO}_2 - F_I\text{CO}_2}{F_{\text{ET}}\text{CO}_2}, \quad (15)$$

where $F_{\text{ET}}\text{CO}_2$ and $F_I\text{CO}_2$ are the CO_2 fractions in the end tidal and inspired air, respectively, as obtained from the experiment.

The fractional O_2 content released by the reagent is determined by Equation 16, where O_2 emission by the reagent is supposed to be proportional to the CO_2 absorption by the reagent:

$$R_{O_2} = k_{O_2} \times R_{CO_2} . \quad (16)$$

The oxygen emission coefficient is calculated based on experimental data:

$$k_{O_2} = \frac{F_I O_2 - F_{ET} O_2}{F_{ET} CO_2 - F_I CO_2} , \quad (17)$$

where $F_{ET} O_2$ and $F_I O_2$ are the O_2 fractions in the end tidal and inspired air, respectively, obtained from the experiment.

2.4. SIMULATION PARAMETERS

The O_2 and CO_2 volumes within the lung tissue compartments were estimated by using Equations 8 and 9 and the solubilities and affinities presented in [12]. The partial pressures of gas i in arterial and venous blood are listed in Table 1.

Table 1

Parameters adopted for the test subject

	O_2	CO_2	
Lung compartment	$M_{LO_2} = 0.62 \text{ L}$ $P_{aO_2} = 100.00 \text{ mmHg}^*$ $\alpha_L = 0.40$ $\alpha_{bl} = 0.02$ $F_{0alvi} = 0.147$	$M_{LCO_2} = 0.50 \text{ L}$ $P_{aCO_2} = 40.00 \text{ mmHg}^*$ $\alpha_L = 0.77$ $\alpha_{bl} = 0.57$ $F_{0alvi} = 0.053$	$V_{0alv} = 3.0 \text{ L}$ $V_{LT} = 1.0 \text{ L}$ $V_{Lbt} = 0.6 \text{ L}$ $V'_{AE}/Q = 1.1$
Tissue compartment	$M_{TO_2} = 0.89 \text{ L}$ $P_{vO_2} = 34.65 \text{ mmHg}^*$ $\beta_T = 1.4 \times 10^{-3} \text{ mmHg}^{-1}$ $\beta_{blt} = 0.9 \times 10^{-4} \text{ mmHg}^{-1}$	$M_{TCO_2} = 14.33 \text{ L}$ $P_{vCO_2} = 45.57 \text{ mmHg}^*$ $\beta_T = 4.1 \times 10^{-3} \text{ mmHg}^{-1}$ $\beta_{blt} = 6.6 \times 10^{-4} \text{ mmHg}^{-1}$	$V_{CT} = 64.0 \text{ L}$ $V_{cbl} = 4.4 \text{ L}$

* the initial values of the gas concentration in blood were estimated using Hill's equations.

Note: F_{0alvi} = gas fraction in alveolar air; P_{aO_2} = arterial O_2 tension; P_{vO_2} = venous O_2 tension; P_{aCO_2} = arterial CO_2 tension; P_{vCO_2} = venous CO_2 tension

The blood flow velocity Q was set to 8.00 L/s. The O_2 consumption rate (J_{O_2}) in the tissue and the CO_2 emission rate (J_{CO_2}) were set to 592 ml/min and 470 ml/min, respectively, as measured for the test subject. The basic parameters of the two model compartments, adopted for the test subject from relevant references, are listed in Tables 1 and 2.

Table 2

Experimental parameters of the test subject used as the input parameters in the simulation

Parameter	Numeric value	Unit
V^a	14.5	L/min
V_T^a	0.85	L
V_{DC}^b	0.246	L
T_{BC}^a	3.6	s
k_{CO_2}	0.99–1.25	–
k_{O_2}	0.96–0.98	–
RQ	0.85–0.95	–

^a mean values of the ventilation parameters obtained from the experiment. The sample includes 21 parameters values, while breathing through the SCSR.

^b measured parameter using the helium dilution technique (VIASIS Master Screen, Jaeger, Germany).

Note: RQ = respiratory exchange ratio; V = alveolar ventilation; V_T = tidal volume

The individual ventilation reactions of the test subject were supposed to be the same as those obtained in [13] for subjects of the same sex and weight.

Experimental and simulation studies were performed assuming the following initial conditions: the total volume of all gases, excluding dissolved gases in blood and tissues but, including the gases in completely deflated SCSR bag, pipes, cassette containing the regenerative cartridge, and gases in alveolar volume, the physiological respiratory dead space was 8 L. The O_2 concentration was 21.2%, the CO_2 concentration was 0.11%, the temperature was 27°C, and the total gas pressure was 760 mmHg.

In the experiment the test subject breathed with the SCSR device for 115 min, the simulation modeling was also executed for 115 min.

As per the experimental data, the inhaled air was gradually heated from 27°C to 37°C by the heat-producing chemical reaction in the reagent. In the mathematical model the temperature function was depicted as a linear function of time.

In the experiment the valve actuation was triggered by 768 mmHg pressure, reducing the pressure to the environmental air pressure of 760 mmHg. During the first 780 s of respiration using the SCSR device, the reagent was warmed up to the steady-state condition; consequently k_{O_2} and k_{CO_2} obtained using Equations 14 and 15 were transient. After the warm-up period, the regenerative cartridge absorbed 98% of the CO_2 expired by the subject ($k_{CO_2} = 0.98$), and O_2 was released at a volume proportional to the absorbed CO_2 volume with a proportionality factor $k_{O_2} = 1.15$. These transient and steady-state values of k_{O_2} and k_{CO_2} were used as the input parameters for simulation.

2.5. NUMERICAL PROCEDURE DETAILS

All of the simulations were performed in MATLAB Simulink R2017b (2017, Mathworks, USA) using the automatic solver with a fixed step size of $\Delta t = 0.01$ s for numerically integrating the set of differential equations.

Therefore, the mathematical model was described by a closed equation system consisting of 10 ordinary differential equations and 21 algebraic equations.

2.6. EXPERIMENTAL PROTOCOL

A normal 34-year-old male volunteer (weight: 80 kg, height: 180 cm) without a history of lung disease and no experience breathing with an SCSR device was selected to examine the model. Before the study, informed consent was obtained from the test subject. The gas flow was measured using an ultrasound gas flow meter (Moscow State Mining University, Russia). The O₂ and CO₂ concentrations were registered by a gas analyzer (MPR6–03, Triton Electronics LLC, Russia). The experimental protocol included 15 min of normal breathing using room air, breathing through the SCSR for 115 min, and breathing using room air for 2 min. SCSR “ShC-30” (Roshimzaschita Corp. JSC, Russia) was selected for testing. The experimental protocol was approved by the bioethical commission of IMBP RAS.

3. RESULTS

Figures 1 and 2 show the F_{O_2} and F_{CO_2} time patterns during the 115 min period of breathing with the SCSR device. In the experiment and simulation, O₂ gradually accumulated in the system and replaced other gases. These dynamics can be explained by the intensive regeneration of chemically bound O₂ during the first 780 s. The simulated and experimental curves agreed well; *e.g.*, the simulated and experimental concentrations achieved constant values simultaneously.

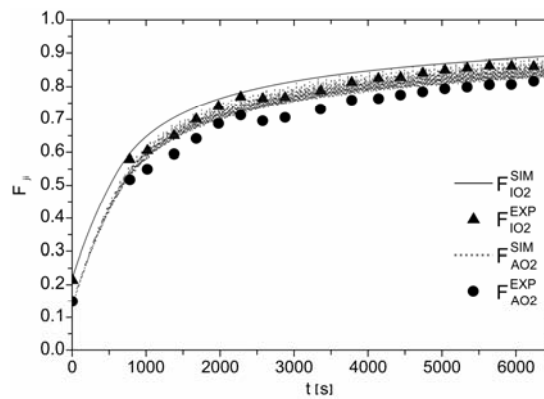


Fig. 1 – Simulated ($F_{IO_2}^{SIM}$) and experimental ($F_{IO_2}^{EXP}$) oxygen gas fractions within the SCSR device, simulated ($F_{AO_2}^{SIM}$) and experimental ($F_{AO_2}^{EXP}$) – oxygen gas fractions in the expired gas.

The experimental and simulated data are presented as obtained in the experiment and as computed in the numerical procedure, respectively.

The CO₂ concentration within the SCSR did not exceed 0.3%, and excessive CO₂ was absorbed by the reagent, whereas the CO₂ in the alveolar space gradually achieved a constant value of approximately 5%.

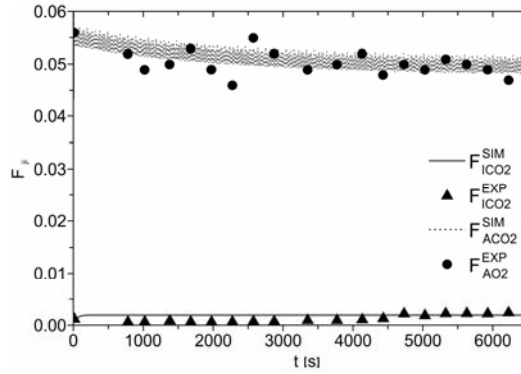


Fig. 2 – Simulated ($F_{\text{ICO}_2}^{\text{SIM}}$) and experimental ($F_{\text{ICO}_2}^{\text{EXP}}$) carbon dioxide gas fractions within the SCSR, simulated ($F_{\text{ACO}_2}^{\text{SIM}}$) and experimental ($F_{\text{ACO}_2}^{\text{EXP}}$) – carbon dioxide gas fractions in the expired gas. CO₂ accumulation from 0.05% up to 0.3% occurs in the SCSR device. The simulated and experimental data agree well.

Figure 3 qualitatively compares the simulated and experimental gas pressure dynamics. The pressure increase in the bag of SCSR device mainly occurred because O₂ generation exceeded the O₂ consumption. Through discharge, each gas was removed from the system proportionally, and the other gases were gradually replaced with the generated O₂.

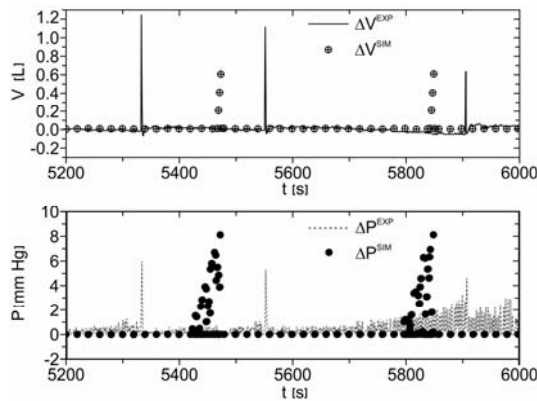


Fig. 3 – Simulated (ΔP^{SIM}) and experimental (ΔP^{EXP}) curves for the gas pressure dynamics as a function of time while breathing through the SCSR device, and gas mixture volume to be released through the valve (computed values (ΔV^{SIM}) and experimental data (a)). Note: ΔP = change in gas pressure per unit time; ΔV = change in gas mixture volume per unit time.

4. DISCUSSION

The proposed model can account for the amplitudes and time patterns of the main respiratory parameters; however, it includes certain simplifications and limitations that will be addressed in future studies. Nonetheless the problem of predicting respiratory gas dynamics during respiration with self-contained self-rescue apparatus was resolved.

The model examination in this study was limited to one subject, one apparatus, and one replication. In future, it is intended to test the mathematical model using a considerably wider sample range with other device models.

This model can be employed for any chemical reagent, described by the O₂ emission coefficient k_{O_2} and the CO₂ absorption factor k_{CO_2} .

In particular, potassium superoxide is a solid chemical that can release O₂ and absorb CO₂ upon reacting with water; thus, the gas-mixture humidity is a key system parameter that characterizes the reagent emission and absorption [14]. Subsequent studies should include the effect of exhaled water vapor in the mathematical model.

5. CONCLUSION

The mathematical model of a biotechnical system consisting of a human cardiorespiratory system and an individual respiratory protective device was developed and examined by comparing the results of simulations with experimental data. The simulated gas accumulation in the compartments corresponded to the experimental observations. Hence, after validation of the model with adequate samples and various breathing devices, the model will be usable for predicting the expected lifetime of an SCSR device based on simulation data instead of real experiments with human test subjects.

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