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CFD Modeling of Breakthrough in Closed Circuit Rebreather Scrubbers

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Abstract: Closed Circuit Rebreathers (CCRs) in SCUBA diving currently have no dependable sensors to indicate when scrubber life has been exhausted with carbon dioxide (CO_2). The kinetics of flow and CO_2 absorption were thus highlighted and the simulation of the chemical reactions within the CCR scrubber is established. A transient model is developed investigating the effects of several key parameters affecting scrubber performance; geometry, wall temperature, velocity, CO_2 absorption, granule size and material selection on breakthrough of the CCR scrubber where breakthrough is defined as the time until the CO_2 exhausting from the scrubber canister is the same as going in. The model is used as an aid to simulate current designs of CCRs; axial and radial scrubbers. The results characterize the sensitivity of the model in regards to the parameters and the behavior of the model is analysed in comparison to previous literature.

Key words: SCUBA, Closed Circuit Rebreathers, Modeling CO_2, Diving applications, Chemical Reaction of CO_2 and Soda lime

INTRODUCTION

The CCR is a type of Self Contained Underwater Breathing Apparatus (SCUBA) used by the diving community, miners and fire fighters. The typical form of SCUBA diving equipment and how one imagines if falls into the common domain of open-circuit SCUBA where exhausted gas or breath is expelled in the form of bubbles from the mouthpiece. Inefficiency occurs through this method as a lot of valuable oxygen gas is wasted as the diver exhales periodically. In order to reduce this inefficiency, the CCR is employed. A typical schematic of CCR operation is shown in Fig. 1 with CO_2 laden exhaled breath leaving the mouthpiece of the diver in which it is absorbed by a chemical compound, generally soda lime, lithium hydroxide or Baralyme(Wang, 1975) in the scrubber, the latter not seen in rebreathers for over 35 years.

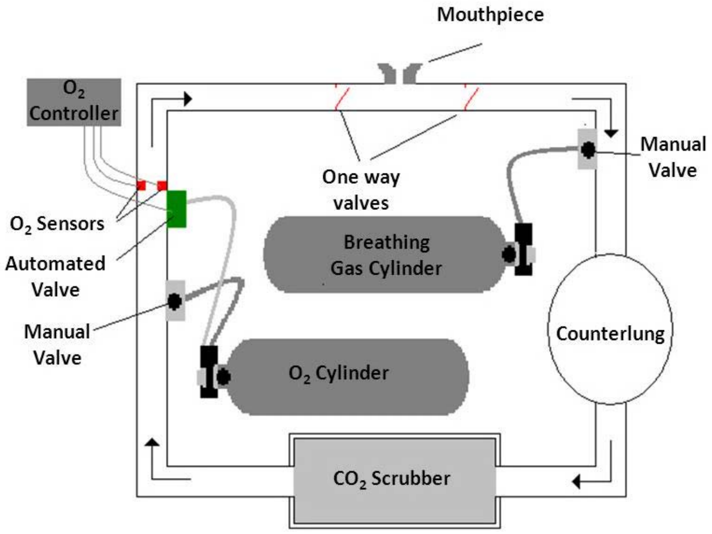

Fig. 1: Closed Circuit Rebreather Schematic. A complete automated system is shown for gas addition. Lines denote direction of gas flow

Oxygenated gas is pumped into the loop to keep the pressure constant to enable the diver to breathe continuously. The benefit of using a CCR is highlighted by three main factors: (i) gas efficiency, (ii) decompression efficiency and (iii) silence or stealth (Deep Life FMECA Report). One of the main dangers currently faced by divers using this equipment is the risk of CO_2 poisoning if the scrubber fails. The scrubber may fail or become less efficient as a result of: (i) complete consumption of the active ingredient, (ii) incorrect packing, sealing or scrubber configuration and (iii) extreme exertion where the diver produces higher amounts of CO_2 (Vann, Pollock, & Denoble, 2007). Disorientation, panic, headache, and hyperventilation are the main

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symptoms of the excess of CO_2 in CCRs (Edmonds, 2002). The development of a transient or dynamic model which characterises/models the chemical reactions which occur between CO_2 and soda lime would greatly enhance the knowledge of these systems. Currently there are two types of designs implemented in CCRs. The most common is an axial design in which exhaled breath is pumped directly through the soda lime which the clean or scrubbed gas exits at the top of the scrubber in Fig. 2 (a) where the shaded section illustrates where the soda lime granules are (Rebreathers Worldwide Website). An alternative but very common design is a radial system shown in Fig. 2 (b) in which the exhaled breath is pumped into the centre stem of the scrubber in which the gas comes into contact with the soda lime radially and following scrubbing, the gas once again enters the breathing loop (Rebreathers Worldwide Website). Exhaled breath passes through the scrubber where the packed soda lime granules absorb CO_2 scrubbing the air. The air passes through the scrubber where each granule can absorb a fixed amount of CO_2 depending on the environmental conditions placed on the scrubber and when this limit is reached the gas passes through unscrubbed until it meets the next unreached soda lime granule.

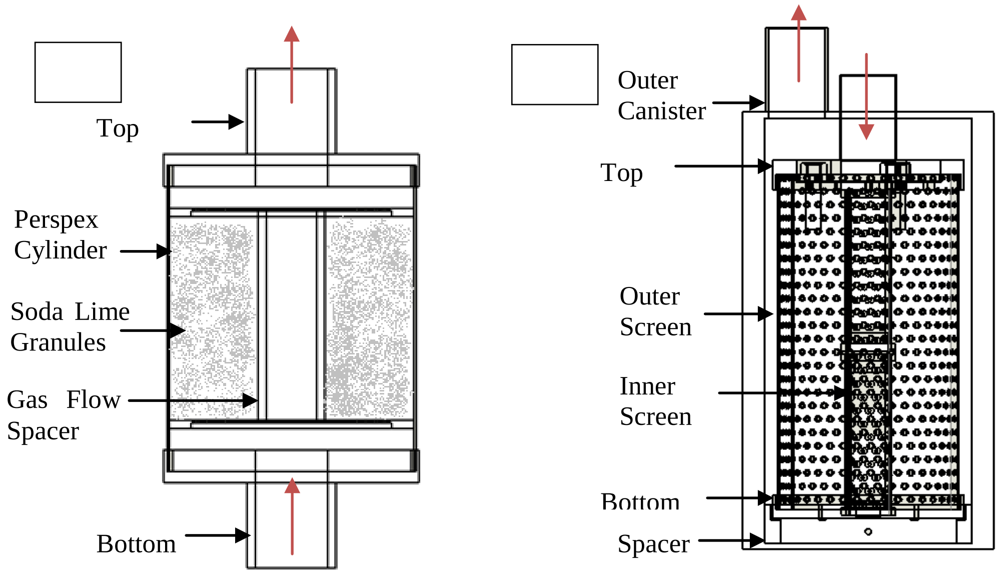

Fig. 2: (a) Axial and (b) Radial CCR scrubber schematics with red arrows denoting gas flow

Until Clarke (Clarke, 2001), the kinetics of absorption in scrubbers was poorly understood. A stochastic method simulating a bed containing a minimum of 200,000 volume elements or cells was employed. Within each cell, the temperature and amount of CO_2 stored for each time increment is defined. The model is constrained by physics as opposed to the chemical properties of the absorbent or CO_2 which means mass and heat transfer are also determined stochastically. The results provide a model simulating CO_2 absorption and thermal fluctuations however the model is limited to the axial designs and no such models of the radial design appear in literature.

Dongsik, Fumin*et al*. (2011) presented work where they analysed imperfect CO_2 removal mechanisms of CO_2 scrubbers. Their work introduced a stochastic model for three CO_2 related rebreather faults: CO_2 bypass, scrubber exhaustion and scrubber breakthrough. They established the concept of CO_2 channeling describing the cause of the faults and present a CO_2 channeling model based on a stochastic process driven by a Poisson counter. In probability theory, a Poisson process is a stochastic process which counts the number of events and the time that these events occur in a given time interval. The work also advances the understanding of breathing dynamics with CCRs and how to maximize performance in terms of breathing and peak to peak pressure however it does not model the chemical reactions occurring inside the scrubber.

Nuckols and Sexton (1983)analysed the use of computer simulation in the design of UBA's. The model is based on a concept of nodes placed in the flow circuit where mass might conceivably accumulate. The model is based on the concentration of mass in Eq. 1; Δm can be expressed in terms of density of gas in the node and the node's volume as,

$$\Delta m = \Delta(\rho V) = \rho \Delta V + V \Delta \rho. \quad (1)$$

Where ΔV is the change in volume during time increment ∂ and $\Delta \rho$ is the change in density during time increment ∂.

Analysis of CCR modeling has highlighted that published work does not model the chemical reactions but employs stochastic methods instead. The aims of the model presented in this paper is to have a simulation where the geometry is an easily changed parameter as well as having a visual user interface in order to gain more information about the internal workings of CO_2 absorption. The feasibility of using chemical properties in a computational fluid dynamic (CFD) analysis is a viable method of modeling CO_2 absorption.

The chemical reaction between soda lime and CO_2 is an exothermic reaction which generates water vapour(M. Nuckols, Purer, & Deason, 1985). This identifies a liquid and gas phase process occurring within the reaction (Olutoye & Eterigho, 2005). Gas absorption occurs when a mixture of gas comes into contact with a liquid for the requirement of dissolving one or more components of the gas mixture into the liquid (Coulson J.M., 1996). Thus the absorption of CO_2 by soda lime reacts chemically with the NaOH component of the liquid phase. Depending on the strength of the coupling between the phases, different modeling approaches can be suggested; homogenous flow models, mixture models, multiphase models or a combination of these (Manninen, Taivassalo, & Kallio, 1996). The homogeneous mixture model is chosen as a suitable model to employ as the flow in this system is laminar and the assumption of the phases moving at the same velocity is valid. To verify the laminar flow, a calculation of the mean particle Reynolds number (Rhodes 1989) is carried out where; ρ is the gas density of CO_2, $\bar{V}$ is the superficial velocity, e is the particle diameter of the soda lime and μ is the dynamic viscosity of CO_2 in Eq. 2.

$$Re = \frac{\rho\bar{V}e}{\mu} \tag{2}$$

A gas density of 1.87kg/m^3 for CO_2, particle diameter of 0.0011m, velocity of 0.0126m/s and dynamic viscosity of 0.0001372kg/ms for standard pressure and temperature conditions gives a mean particle Reynolds number of 0.189 where laminar conditions apply up to Re=10 (Rhodes, 1989).

Assuming CO_2 is a simple gas, Henry's law is applied to describe the equilibrium between vapour and liquid. Literature (Rouhollah Farajzadeh, Barati, Delil, Bruining, & Zitha, 2007; Rouhi Farajzadeh, Zitha, & Bruining, 2009)has used Henry's law in the sequestration/capture of CO_2. Henry's law is applied to describe the equilibrium between vapour and liquid. According to Carrol and Mather (Mather, 1992) a form of Henry's law can be used for modeling the solubility of CO_2 in water for pressures up to 100MPa. Application of Henry's law to calculate CO_2 yields a value 29.41 Latm/mol,

$$p = k_H c. \tag{3}$$

where*p* is the partial pressure of the solute in the gas above the solution, c is the concentration of the solute and $k_H$is a constant.

The reaction between CO_2 and soda lime can be considered a 3-step reaction described by Eq. 4, Eq. 5 and Eq. 6. The first step describes how CO_2 dissolves into water in Eq. 4(Reid, Prausnitz *et al*. 1987).

$$CO_2 + H_2O \rightarrow CO_2(aq). \tag{4}$$

$$CO_2(aq) + NaOH \rightarrow NaHCO_3. \tag{5}$$

Eq. 5 illustrates how the strong base in this case NaOH is not fully consumed but acts as a catalyst in the reaction. This bicarbonate is formed due to the high pH. The final step in Eq. 6 deals with the production of calcium carbonates,

$$NaHCO_3 + Ca(OH)_2 \rightarrow CaCO_3 + H_2O + NaOH. \tag{6}$$

Adding together the three reaction steps, you get the overall reaction in Eq. 7 where the heat release is 16,400 cal/mol of CO_2(Sodasorb Manual 1986).

$$CO_2 + Ca(OH)_2 \rightarrow CaCO_3 + H_2O + \Delta H. \tag{7}$$

MATERIALS AND METHODS

Many factors affecting the performance of CO_2 scrubbers are beyond the control of the designer; for instance, the operational pressure and temperature are usually fixed by the diver's surroundings. Any efforts to operate the scrubber in conditions other than the diver's surroundings would be at the expense of energy, complex designs, and cost. There are several variables which must be taken into account when modeling CCRs such as geometry, wall temperature, velocity, granule size and material selection of the CCR scrubber. The CO_2 laden gas must have an adequate dwell time within the scrubber to allow the process of absorption to occur. This means if the flow rate is too quick, the reaction will fail even if all the other variables are ideal. The paper analyses these factors through a computational fluid dynamic model (CFD) using the chemical reactions discussed in the introduction. The benefits of using a chemical model with a visual user interface are also discussed. An analysis of the chemical reaction between CO_2 and soda lime was undertaken using a computer software package called Ansys CFX 13.0. This package allows the user to simulate flow properties of a given system.

Transient Models:

To analyse CO_2 flow in real time, transient simulations were developed. The geometry for the simulation was a single segment of 1^o degree which is shown schematically in Fig. 3 (a) for an axial scrubber. The full scrubber consists of a canister bed length of 279.4mm and width of 146mm. The geometry of a single segment of 1^o degree is shown schematically in Fig. 3 (b) for a radial scrubber. The full scrubber consists of a canister bed length of 254mm and width of 127mm.

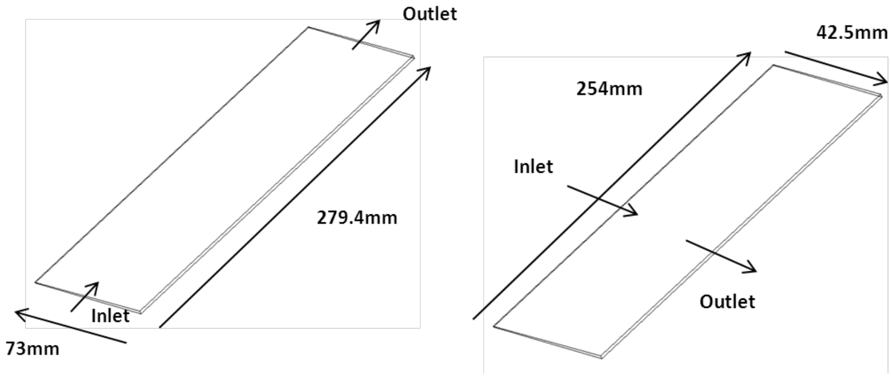

Fig. 3: Schematic of the model axial scrubber slice (a) and schematic of the model radial scrubber slice (b)

Ansys 13.0 contains two main types of errors which may impair the simulation from running or impair the results; (i) in-built CFD errors and (ii) physical errors (National Aeronautics and Space Administration (NASA) Website). In built errors occur within the set-up of the CFD model itself which are the most difficult errors to avoid as they cannot be reduced systematically. Physical errors occur from the assumptions the user defines for the model which in this case is; (i) the CO_2 is absorbed fully without loss until breakthrough, where breakthrough is defined as the time until the canister effluent passes through the soda lime granules unscrubbed, (ii) the CO_2 gas is uniformly distributed throughout and (iii) a constant CO_2 injection rate is employed. Boundary conditions are also employed in the model. The axial scrubber is modeled as a porous media receiving exhaled breath; 5% CO_2, 16% O_2, 78% N_2 and traces of water vapour at a constant inlet velocity of 0.0126m/s. When the composition of exhaled breath passes through this porous media, a series of chemical reactions take place absorbing the CO_2 and producing water vapour and heat. The inlet gas has a static temperature of 25^oC and a boundary condition of atmospheric pressure was set. The porous bed is comprised of spherical granules with a granule diameter of 1.1mm. The following parameters were analysed in the transient simulations (i) inlet flow rate, (ii) granule size or porosity of bed, (iii) wall effects, (iv) outside wall temperatures and (v) material properties of the wall. Each parameter is simulated by holding all other variables constant whilst changing the given parameter in question. Through this the breakthrough of CO_2 is characterized for each parameter in the model where breakthrough is defined as the time taken for full consumption of the soda lime media.

Results:

Impact of CO_2 injection rate on breakthrough:

The CO_2 injection rate is varied in order to analyse this effect on the scrubber system while holding the other variables constant. Four injection rates were used; 1.5 l/min, 3 l/min, 4.5 l/min and 6 l/min and Fig. 4 illustrates the results. Fig. 4 illustrates the four simulated flow rates and the time taken for each flow rate to reach breakthrough. Two effects are visible from the graph; the lower the CO_2 injection rate, the longer it takes for CO_2 breakthrough and the second effect is particularly illustrated between 0 and 500 seconds in Fig. 4. The higher the CO_2 injection rate the greater the level of CO_2 gas breaking through without complete absorption. The reaction between CO_2 and soda lime takes 0.5 seconds to occur, if the gas is too quick passing through the canister, more CO_2 will pass through unscrubbed as the gas is not allowing enough residence time on the soda lime which can attribute to the second effect noticed in Fig. 4. The exhaled breath from the human body is approximately a flow rate 0.5 l/min. Manufacturers use 1.5 l/min because the flow rate travels slow enough to allow the gas to have enough residence time with the soda lime and maximizes the time taken to test the scrubbers. It provides the same dissipation properties throughout the scrubber as one being tested with a flow rate of 0.5 l/min (Navy Manual 1994).

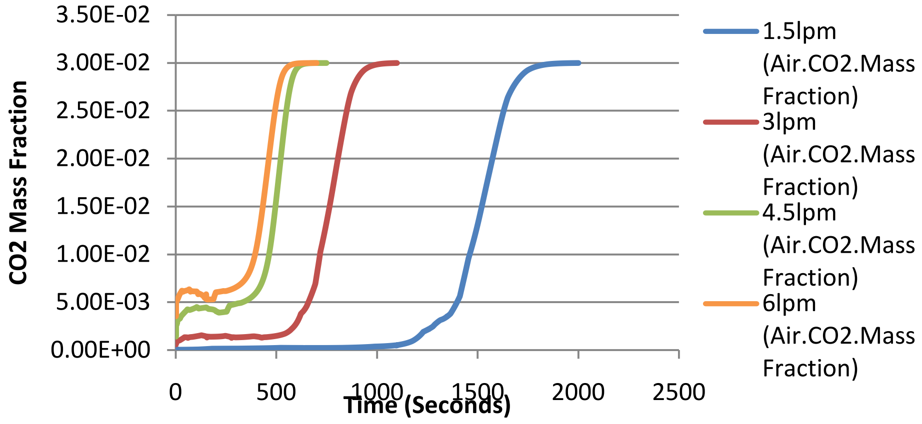

Fig. 4: Transient CO_2 breakthroughs versus time for different CO_2 injection rates in an axial CFD model
Impact of porosity on breakthrough

The morphology of soda lime is an important factor to consider when designing CCR scrubbers. In order to analyse the effect of the soda lime granule on the system different particle diameters were analysed. The first particle diameter is 1.1mm used in the 797 grade of soda lime ("Technical Data Sheet for Carbon Dioxide absorption, Sofnolime for commercial and leisure diving,") and the second particle diameter used was 3.6mm (M. Nuckols, *et al*., 1985), a diameter size used in the technical manual Design Guidelines for Carbon Dioxide Scrubbers. Fig. 5 illustrates the graphical comparison between the two granule particle sizes against CO_2 concentration over 2000 seconds. The first aspect noticeable from Fig. 5 is the smaller the particle size the longer until scrubber breakthrough. The method in which breakthrough occurs for both is different. The 3.6mm size exhibits a vertical breakthrough line as opposed to a slanted profile line from the 1.1mm particle size. This suggests that CO_2 passes through the canister with 3.6mm particles quicker than the 1.1mm granule size due to a greater slope as the smaller granule size offers more resistance to the flow than a larger granule size.

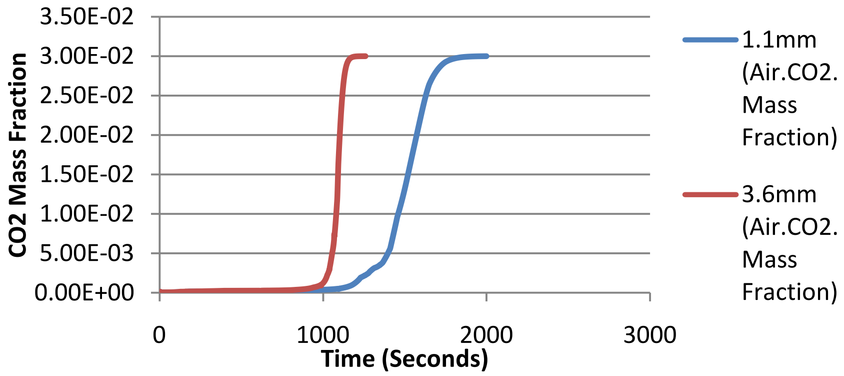

Fig. 5: Transient CO_2 breakthroughs versus time for an axial CFD model comparing granule size

Flow resistance through the canister varies inversely with particle size. That is the finer the pellets, the greater the surface area exposed to air friction. Large particles offer less resistance but have the disadvantage of providing a smaller total surface area for reaction. In order to analyse the results in Fig. 5 in greater detail, the distributions of CO_2 concentration in the visual segment simulated is used in Fig. 6. In the analysis of the 3.6mm particle size, Fig. 6 (b) illustrates gas flowing from bottom to top and channeling at the wall with a curved reaction front profile. The larger the particle size, the easier gas concentration travels up the walls. The effect the wall has on the absorption properties is known as edge effects. Fig. 6 (a) illustrates the 1.1mm particle size where no edge effects are present. The graphs characterize the reaction active zones and it is seen the 1.1mm has a much smaller active zone than the 3.6mm. The narrower the reaction zone the less CO_2 concentration is seen breaking through the system due to the smaller granule size. A curved and larger reaction active zone is seen in Fig. 6 (b) where the smaller surface area allows gas to passmore freely to next line of granules before the initial active layer is consumed i.e. gas passes to the yellow band before the orange band is at complete consumption.

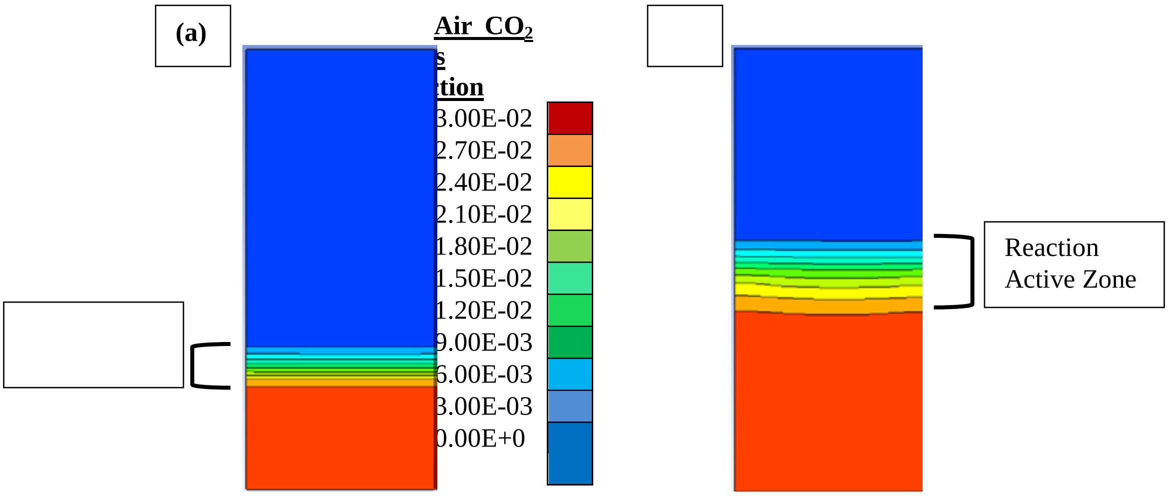

Fig. 6: Axial distributions of CO_2 concentration for (a) granule size of 1.1mm and (b) granule size of 3.6mm

Outside temperature effects on breakthrough:

A CCR may be placed in waters of various temperatures and as stated in the introduction the reaction between soda lime and CO_2 is temperature dependent. To analyse the effect of the outside temperature on the reaction occurring within the scrubber, a boundary temperature will be placed on the walls of the scrubber. These temperatures represent possible temperatures of the water to which the scrubber may be subjected to. Two temperatures are used, a wall temperature of 20°C and one at -1°C. Fig. 7 graphs the results of the two temperatures. Very little difference is seen except the scrubber with a wall temperature of -1° takes longer to reach breakthrough.

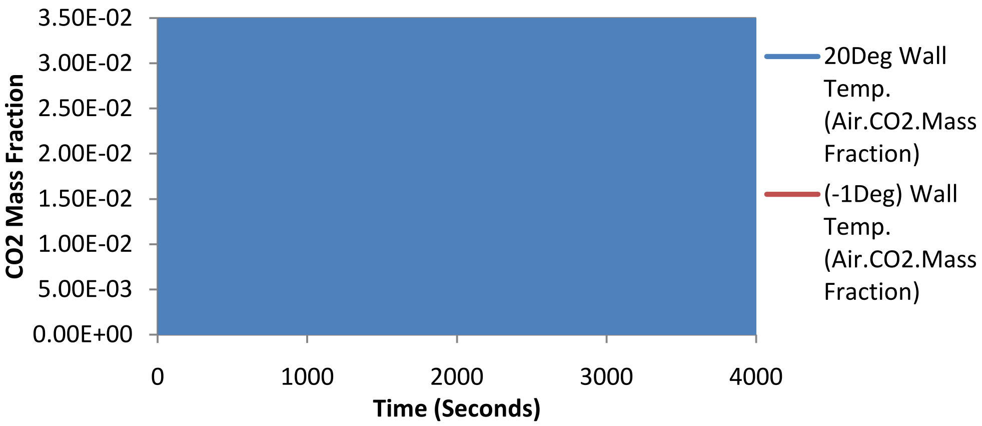

Fig. 7: Transient CO_2 breakthroughs versus time for an axial CFD model comparing the effect of wall temperature on the system

Fig. 8 illustrates the comparison of the wall temperatures through the simulated scrubber model on CO_2 breakthrough. Though slight, Fig. 8 (b) illustrates CO_2 channeling or edge effects occurring on the wall of the simulation where the boundary condition was set at -1°C. CO_2 gas passes easier without absorption along the walls rather than the level reaction zone moving through Fig. 8 (a). An effect to the scrubber due to temperature is shown which corresponds to existing literature. The absorption rate of chemical absorbers is directly related to the bed temperature (Cook, 1972). Scrubber testing has shown that absorption capacities are decreased in cold settings (-1°-4°) (Aroonwilas, Chakma, Tontiwachwuthikul, & Veawab, 2003). The variable of temperature is difficult to maintain due to the inter-relation of bed temperature and moisture level: a high bed temperature is more inclined to dry out the absorbent and impede the completion of the reactions and a low temperature affects the reaction from taking place (M. Nuckols, *et al.*, 1985).

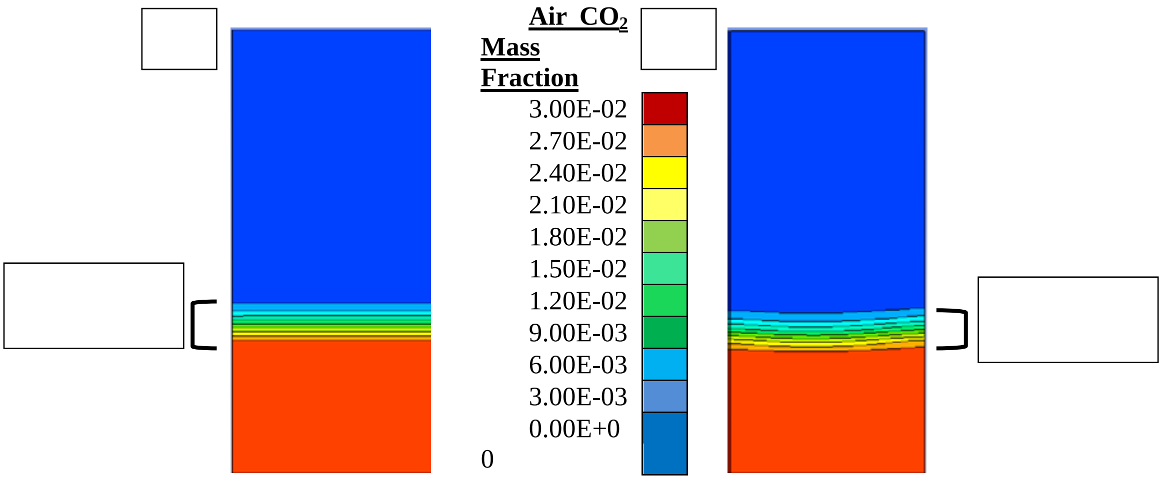

Fig. 8: Axial distributions of CO_2 concentration for (a) wall temperature of 20°C and (b) wall temperature of -1°C

The CFD simulated model also illustrates the comparison of the internal bed temperatures occurring within the scrubber. Fig. 9 (a) shows the bed temperature of a scrubber with a 20°C wall temperature. Similar to the reaction active zone, the bed temperature exhibits a smooth/level profile with a consistent moving temperature front. This is due to the optimum conditions for the reaction to occur. Fig. 9 (b) illustrates the bed temperature of the scrubber with a -1°C wall temperature. This exhibits a contoured moving temperature front with the optimum temperature occurring in the center of the scrubber. This corresponds to the active reaction zone in Fig. 8 (b) where the least amount of channeling is seen in the center of the scrubber. Channeling of CO_2 occurs along the walls where the temperature is at its lowest.

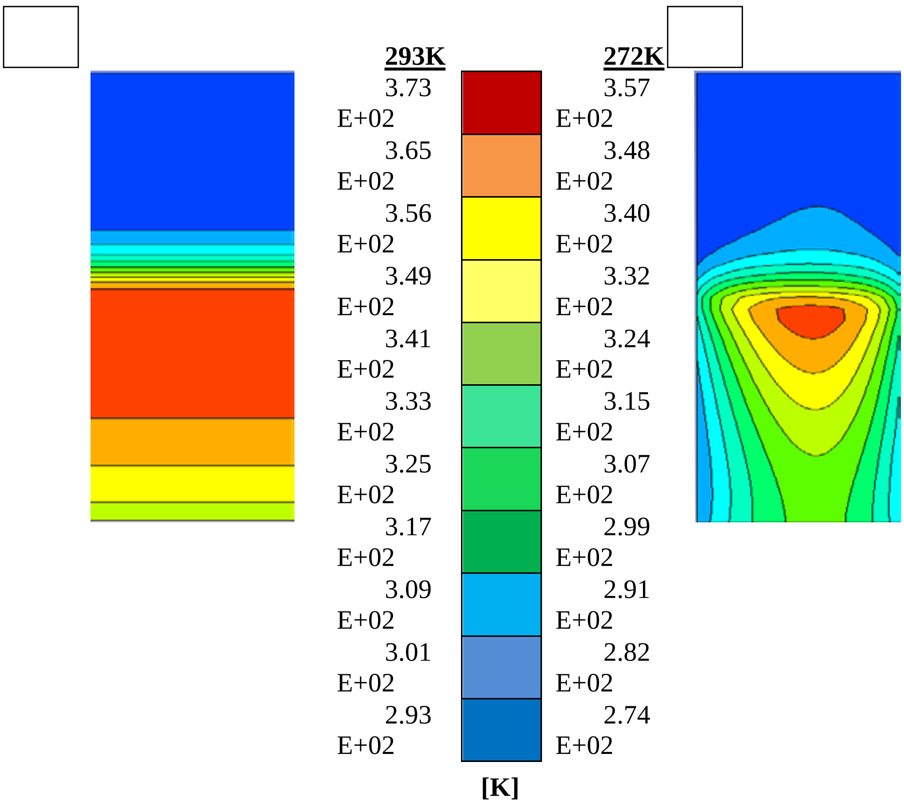

Fig. 9: Axial distributions of bed temperature for (a) wall temperature of 20°C (293K) and (b) wall temperature of (-1°C) (272K)

Effect of material properties of the wall on CO_2 breakthrough:

The material of the wall in the model can be specified to represent certain materials using the wall heat transfer coefficient. This allows the comparison of the effect of heat transfer between plastic and steel, the two materials being analysed in this paper. The material properties of the wall are important due to the high temperatures and corrosive environment produced by the chemical reactions within the scrubber (Klos, 2008). Plastic is a suitable material as it possesses low absorption qualities in terms of the humidity and is chemically resistant to solvents and neutral chemicals (Plastics International Datasheet 150). Stainless steel is an ideal material choice as it would not corrode easily (ATI-Technical Data Sheet Website). Both these materials are also used in the experimental design section where plastic makes up the axial scrubber and stainless steel is predominantly used in the radial scrubber.

Fig. 10 graphs the CO_2 mass fraction over time for a model with the heat transfer properties of 4.0Wm^2/K representing a polycarbonate plastic and 25Wm^2/K representing a 304 stainless steel grade.Fig. 10 illustrates the stainless steel exhibits the exact same CO_2 levels as the polycarbonate model showing no difference in the performance of the scrubber with these materials.

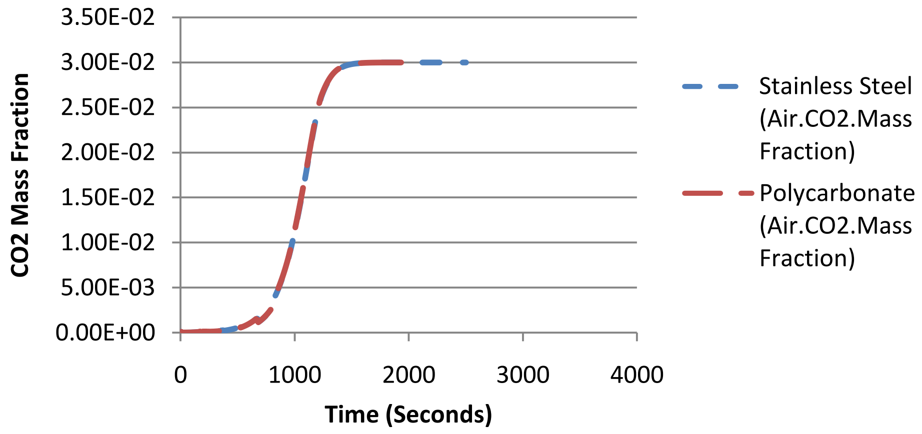

Fig. 10: Transient CO_2 breakthroughs versus time for an axial CFD model comparing the effect of material selection of the scrubber

The internal bed temperatures of each of the scrubbers are compared in Fig. 11. The sensitivity of the CFD simulation is more observed here as the plastic material is a better insulator than the stainless steel material which is picked up in the CFD simulation.

Radial Scrubber Canister Results:

The variations in granule size and material selection will generate similar results in both the axial and radial scrubber. Due to the change in geometry, the flow rate and outside wall temperature will show behavioral differences depending on which style of scrubber is simulated. The velocity of the gas is lower passing through the granules in the radial scrubber than the axial scrubber even though the inlet flow rates are the same. The scrubber path for the radial scrubber is 42.5mm. The volumetric flow rate is constant so the area velocity decreases rapidly. Fig. 12 graphs the variation in CO_2 injection rate; 1.5 l/min, 3 l/min, 4.5 l/min and 6 l/min for the radial scrubber. Similarly to the axial scrubber the higher the injection rate the greater the level of CO_2 gas breaking through without complete absorption. In comparison to the axial scrubber for the same CO_2 injection rate lower amounts of CO_2 are breaking through between 0 and 500 seconds. The radial design copes better with higher CO_2 injection rates than the axial. In order to keep the CO_2 content in both the radial and axial scrubbers closer to 0 a slower flow rate is required.

The radial design has an outside canister around the scrubber which acts as an insulator to it. The temperature of the outside wall or water temperature will affect this style of scrubber less than an axial one. Fig. 13 illustrates the CO_2 breakthrough for a radial canister with an outside wall temperature of -1^{o}C and an outside wall temperature of 20^{o}C. A small difference is visible in terms of CO_2 breakthrough where the 20^{o}C canister performs marginally better.

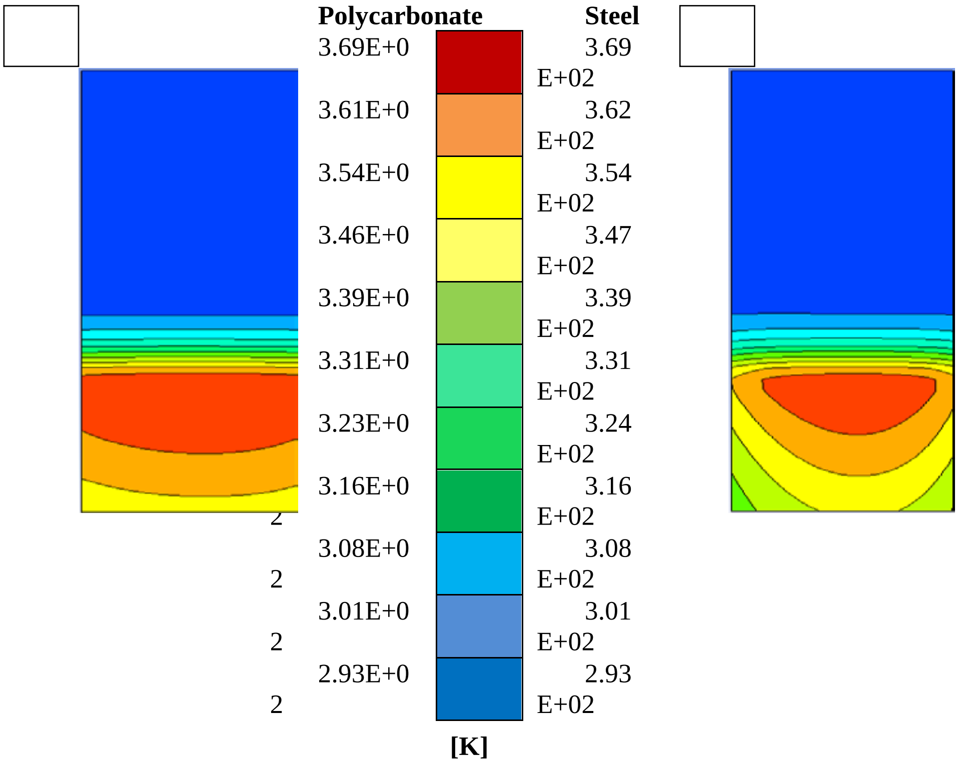

Fig. 11: Axial distributions of bed temperature for (a) polycarbonate material and (b) stainless steel material

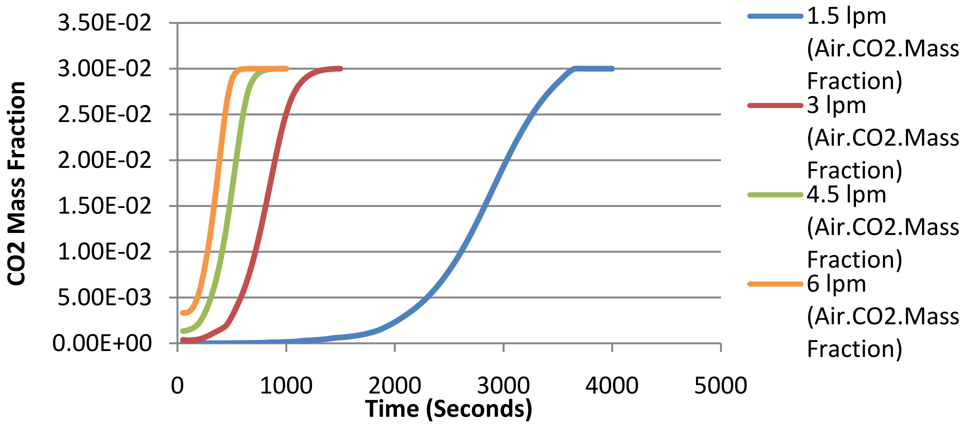

Fig. 12: Transient CO_2 breakthroughs versus time for different flow rates in a radial model

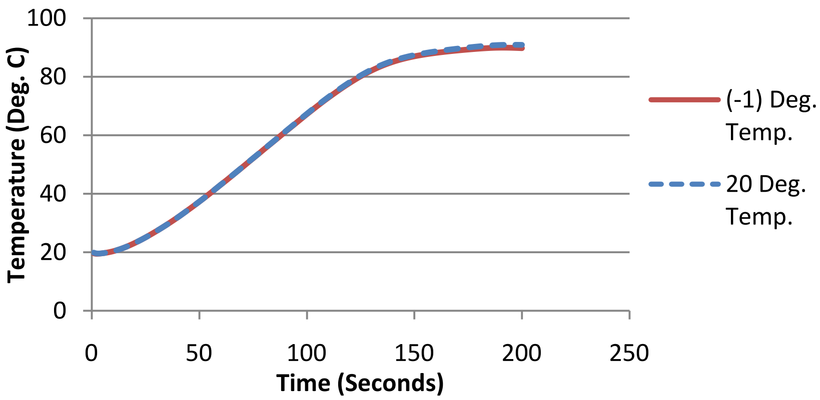

Fig. 13: Transient CO_2 breakthroughs versus time for a radial CFD model comparing the effect of wall temperature on the system

The simulated model in Fig. 14 (b) shows a similar channeling or edge effect that was seen when the axial model was analysed. Conduction is occurring with the water on the top and bottom of the model. This once again validates the theory that low temperatures will have an effect on the absorption properties of the scrubber.

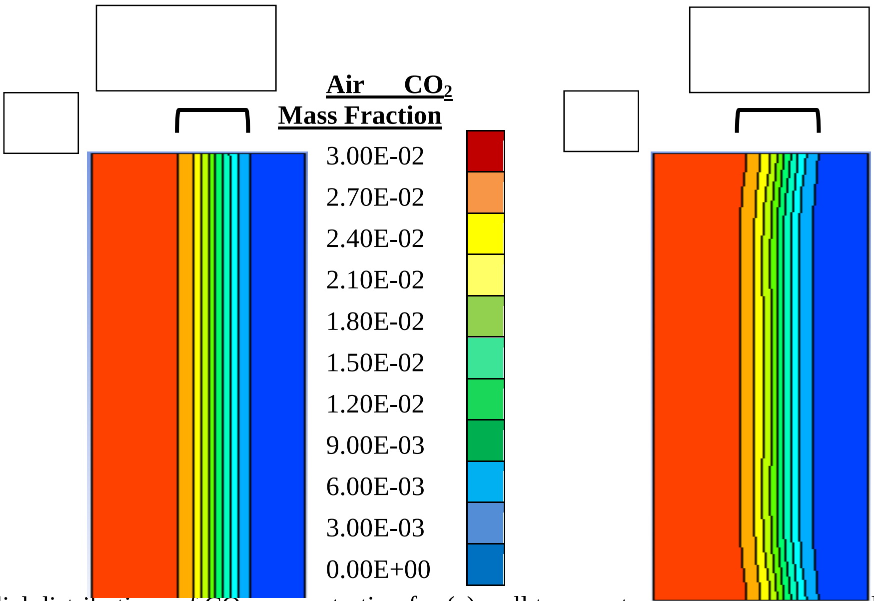

Fig. 14: Radial distributions of CO_2 concentration for (a) wall temperature of 20°C and (b) wall temperature of -1°C

Due to the length of the CO_2 moving front in Fig. 15 (b), the high temperatures occurring as a result of the chemical reaction can be maintained in the center of the scrubber which is further validated in the simulated temperature model. In comparison to the axial scrubber under the same conditions, the radial maintains a maximum temperature of 90°C (263K) whilst the axial has a maximum temperature of 84°C (357K). The radial design is a better insulator when it comes to the outside wall or external temperature.

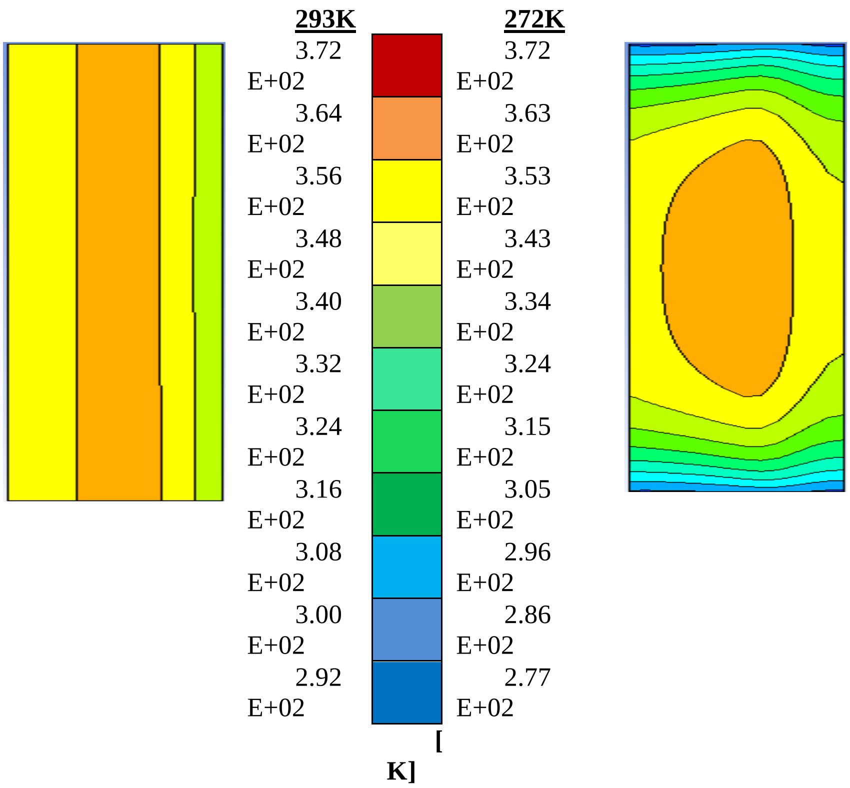

Fig. 15: Radial distributions of bed temperature for (a) wall temperature of 20°C (293K) and (b) wall temperature of -1°C (272K)

Discussion:

The paper presented a mixture model using the chemical reactions between soda lime and CO_2 as an alternative simulation technique to analyse the properties of a CCR scrubber. The following properties were altered and analysed as a means of showing the capabilities of the model (i) CO_2 injection rate, (ii) granule size or porosity of bed, (iii) outside wall temperature, (iv) material properties the of wall and (v) geometry. Each parameter was analysed and in the cases of (ii)-(v) the need for a graphical representation in scrubber kinetics was verified. The models behave using all the essential chemical factors between soda lime and CO_2. The analysis of the CO2 injection rate highlighted the importance of the parameter to the scrubber system. Both the axial and radial analysis showed where there is a higher CO2 injection rate, the faster breakthrough occurs. Higher amounts of CO_2 are seen breaking through in the earlier stages of the 4.5 and 6 l/min for the axial scrubber in comparison to the radial scrubber where little increase is seen. The porosity of the soda lime bed analysed the effect of changing the particle diameter on the system in which two effects became prominent. The first effect illustrated the smaller the diameter the more surface area available for the CO_2 gas to be absorbed and vice versa for the larger the diameter. Fig. 6 (a) and (b) illustrate the difference in the reaction zone between both granule sizes. It becomes apparent the smaller the reaction zone the more efficient the scrubber. Edge effects were also seen in Fig. 6 (b). The larger the particle diameter the more gas volume within the scrubber which allows gas to travel with less resistance up the wall. Temperature effects have been analysed throughout the paper, lower temperatures affect the absorption of CO_2. Temperatures do not exceed 100^oC in the scrubber canister due to when the reaction occurs the water/humidity will start to boil and give off vapour. The consequent absorption of latent heat effect will prevent the temperatures rising above 100^oC as seen in the experimental program.

A versatile model simulating chemical reactions within a CCR canister for both the axial and radial scrubber design has been shown to be capable of analysing the design parameters of interest in this paper.

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