



Modelling of adsorption technologies for controlling indoor air quality

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Abstract

Technologies for control of indoor air quality are very important to ensure that health and comfort conditions are attained in closed environments. The indoor air quality market is fertile ground for adsorption technologies, both at larger industrial scale and for residential uses. The common strategy to design adsorption technologies considers constant inlet conditions, while for most indoor air control applications, the inlet conditions will change because of the partial removal of the contaminant. This work presents a generic modelling approach, where the adsorption technology is coupled with the indoor environment to be controlled. This approach enables a tailored and more accurate process design and additionally, it can also assist in the physical location of the removal unit and sensors to control its operation. Two different examples of application of this methodology are provided: control of CO₂ in tightly closed environments and "peak shaving" of water vapor in bathrooms.

Keywords Process modelling · Indoor air quality · Adsorption · Carbon dioxide · Water

1 Introduction

Human beings rely on clean air for survival. The existence of pollutants in the air surrounding us is a problem that brings sensorial discomfort, can deteriorate health and in worse cases, carries life risks. Control of indoor air quality (IAQ) is a very important topic provided that humans are concentrated in closed environments for education, work, recreation, etc. [1, 2].

The type and quality of pollutants, their concentration and emission rate are extremely diverse and depends on many factors [3]. In households, the most common pollutants with health risks are volatile organic compounds [4], formaldehyde [5–7] and in some cases, ozone, radon, carbon monoxide and tobacco smoke [8]. Radon is the first cause of lung cancer among non-smokers [9]. The lack of control of relative humidity inside some areas of the house, particularly in the bathroom, can promote the formation of mold which produce allergens and irritants that are harmful to some people

[10]. In households, the humidity generation is not constant and comes in peaks when events like shower or cloth drying happens. In commercial buildings the contaminants are the same, but in many cases there is some more specificity: i.e. there can be plenty of CO and CO₂ in underground parking.

In underground parking of commercial and recreation buildings, important contaminants are carbon monoxide, nitrogen oxides and other products originated from transportation. In the other levels of such buildings, carbon dioxide can be problematic. Human beings exhale carbon dioxide and water in every breath [11, 12]. Accumulation of carbon dioxide in closed environments has already been acknowledged and reported [13] [14]. The problem is increased in tight environments, like spaceships [15], Ebner et al. 2009; [16] or submarines [17], [18] where air evacuation is not an option. In those circumstances, without a CO₂ removal device, the carbon dioxide exhaled can accumulate until a point where is dangerous to health. It has been previously reported that one astronaut emits around 42 g of CO₂ per hour [19]. Accumulation of CO₂ over 3% is already a health problem, while accumulation over 5% may possess life risks [20]. In such tight environments with a fixed crew, the generation of CO₂ is continuous, and its amount can have variations depending on the activity level of the personnel. In buildings, the generation of CO₂ depends on the amount of people present at a given fraction of time [21].

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The legal requirements to comply healthy standards make the IAQ a multi-million market for different technologies for gas filtration and cleaning as well as for measuring devices. Estimating the market value is difficult because it depends very much on the items accounted: reported values range from 159 million USD [22] up to over 10 billion USD [23]. Major industrial players in the market are TSI, Lennox, Thermo Fisher Scientific, 3 M, Honeywell, Aeroqual, Tedyne, Trane, Carrier, Dyson, PPM, etc. The market share of large installations for industrial and commercial buildings is over 70% while the rest covers residential buildings.

To avoid accumulation of undesired substances in indoor environments, technologies for air cleaning or air filtering are energy efficient solutions. There are several technologies based on different physicochemical principles that can be used. Selective adsorption of targeted substances in porous adsorbents is an interest possibility [24, 25]. Adsorption processes are used for different polishing applications and are industrially acknowledged by their low energetic requirements. Moreover, adsorption units are known for presenting low maintenance requirements with adsorbents that are (or that can be tailored to be) environmentally friendly [26]. Utilization of adsorption technologies for air filtering has indeed shown that they can contribute to significant savings of energy when compared with standard ventilation systems [27] [21]. The adsorption equipment used in IAQ applications does not need to follow the traditional fixed-bed columns arrangement, the desiccant rotating wheel for control of temperature and relative humidity in commercial buildings commercialized by Munters AS is a good example of technologies designed to operate with low pressure drop. Equipment can even be tailored to remove one or multiple components by using different layers of adsorbents [28].

The vast majority of the adsorption processes are designed with constant feed conditions [29, 30]. For designing an adsorption system for indoor air control there are two factors that should be considered and are, for simplicity, commonly ignored:

1. At least during some parts the operation, the rate of generation and the rate of adsorption will not be the same, so the rate of change of the component to be removed from the indoor volume should be accounted for, and
2. An optimized control system for the adsorption process should account for possible distributions of the contaminant in the indoor space, which implies that concentration should be considered as a function of the spatial location and an optimal location of the unit could be found.

An adsorption process can be designed without considering these two factors. However, in terms of process intensification, a more accurate design can result in a unit with a

smaller size (and weight) and smaller power consumption. This work presents a mathematical model that solves the variation of given species in an indoor volume after integrating an adsorption technology for air purification. A distinctive feature of this model is that the inlet concentration of the component entering the fixed bed adsorption technology is changing with time as the component is being removed, or until a cyclic steady state is achieved.

The generic mathematical model is presented and used to simulate two different cases with different operation regimes: (a) continuous carbon dioxide removal from a closed environment (like a spaceship or a submarine) and (b) removal of water vapor peaks generated in bathrooms, termed here as “peak shaving”. In this publication, the regeneration of the adsorbent is not considered because the main focus is to show how the concentration of the contaminant changes in the control volume under different circumstances. This work also shows how efficient model-driven design can assist in overcoming thermal effects produced from the fast adsorption of targeted components, both in terms of process design but also in customization of adsorbent shaping.

2 Mathematical model

Adsorption processes rely on the use of a selective material to remove one or more components from a fluid phase. After equilibrium between fluid and adsorbed phases is achieved, the adsorbent should be regenerated. For this reason, adsorption processes are transient and comprise different steps: adsorption, required regeneration steps and other steps to reestablish the system. When the adsorbent is packed in columns, the mathematical model of the columns is given by a set of partial differential equations with respect to time and at least one spatial dimension. While in certain circumstances only the mass balance can be used, the energy released by the adsorption phenomenon causes local temperature increase, and thus the energy balance should be solved simultaneously. Moreover, when the adsorption process is applied to a gas phase, the momentum equation [31, 32] or a simplification like the Ergun equation should be used to describe the pressure drop of the system caused by the bed(s) [33]. The system is solved with boundary conditions that change over time depending on the different steps used (adsorption, desorption, purge, etc.).

A simplified scheme of an adsorption process integrated in a closed environment to selectively remove one or more components is given in Fig. 1. Note that for simplicity, the volume of the adsorption process (V_{ads}) is separated from the indoor volume (V_b), but in most situations, the adsorption process will be placed inside the closed environment. It should also be noted that in this scheme, the necessary elements to regenerate the adsorbent are not considered.

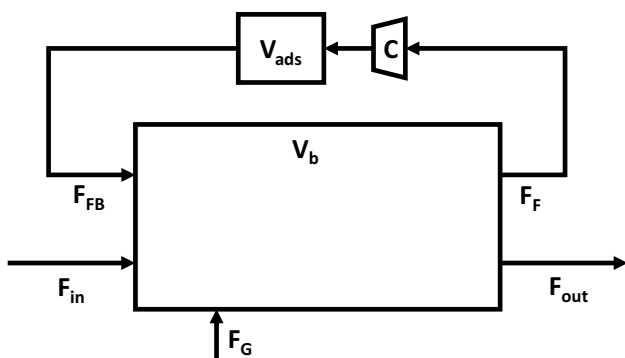


Fig. 1 a Scheme of the different inlet and outlet streams used for modelling the air purification of an indoor volume (V_b) by an adsorption technology (V_{ads})

The regeneration can be done by pressure reduction using a vacuum pump, or by temperature increase, either using a hot fluid or electricity [34]. The electricity can be used to directly heat the adsorbent or to power an electrical resistance that will heat the fluid used for regeneration. For certain operations (removal of VOCs), a thermal oxidation step may be more appropriate.

A mass balance for the component i (to be removed) taken in the indoor volume is given by:

$$F_{in,i} + F_{FB,i} + F_{G,i} - (F_{out,i} + F_{F,i}) = \frac{\partial n_i}{\partial t} \Big|_{V_b} \tag{1}$$

where $F_{in,i}$ and $F_{out,i}$ are possible inlet and outlet streams to the system, respectively, $F_{F,i}$ is the stream that will be routed to the adsorption unit, $F_{FB,i}$ is the stream returning to the closed volume, $F_{G,i}$ is the flowrate of that component i that is generated in the indoor volume and $(\partial n_i / \partial t |_{V_b})$ is the accumulation term in the indoor volume.

Using a similar rationale (“Inlets” – “Outlets” = “Accumulation”), the accumulation in the adsorption process $(\partial n_i / \partial t |_{V_{ads}})$ is calculated by:

$$F_{F,i} - F_{FB,i} = \frac{\partial n_i}{\partial t} \Big|_{V_{ads}} \tag{2}$$

For cases where the system is completely closed, $F_{in,i} = F_{out,i} = 0$. In such cases, replacing Eq. (2) in Eq. (1) and rearranging, we obtain:

$$\frac{\partial n_i}{\partial t} \Big|_{V_b} = F_{G,i} - \frac{\partial n_i}{\partial t} \Big|_{V_{ads}} \tag{3}$$

This equation can be used to depict different scenarios to describe how an adsorption technology can be used for indoor air purification:

1. This equation allows to establish the baseline scenario where only air recirculation and no adsorption technology is used and where $\partial n_i / \partial t |_{V_b} = F_{G,i}$
2. In circumstances where a continuous removal of a given component is targeted, the purification technology should be designed to avoid accumulation of such component in the indoor volume and the technology should be designed to achieve $\partial n_i / \partial t |_{V_{ads}} = F_{G,i}$. An example for such conditions is CO₂ removal from tight environments, like spaceships and submarines.
3. Another possible application of an adsorption purification technology is to remove or “shave” peaks of a certain contaminant. If the technology starts after the generation ceased, then $\partial n_i / \partial t |_{V_b} = -\partial n_i / \partial t |_{V_{ads}}$. This scenario is closer to the case of water removal from bathrooms during or after shower, or when painting locations with poor ventilation [35, 36]. In this scenario, having a model where the indoor volume is directly coupled with the adsorption process is an advantage

To model an adsorption unit coupled to an indoor volume, different equations should be used to calculate each of the terms in Eqs. (1) and (2). The generation term in some cases is fixed or constant while in some cases is intermittent or changes with time [21]. The generation term is very important since it has a major role in sizing of the equipment. The accumulation terms (in the indoor volume and in the adsorption technology) should be calculated with independent equations describing the behaviour in the indoor volume (type of mixing, etc.) and also the type of adsorption technology (batch, fixed-bed, etc.). In this work, a perfectly stirred volume is used for describing the indoor volume where the contaminant concentration has to be controlled. A packed bed adsorption technology is used to remove such contaminant.

The mass balance for the perfectly mixed indoor volume is:

$$\frac{\partial n_{i,b}}{\partial t} = \sum_{j=0}^{inlets} F_{i,j} - \sum_{k=0}^{outlets} F_{i,k} \tag{4}$$

where $n_{i,b}$ is the number of moles of component i in the indoor volume and $F_{i,j}$ and $F_{i,k}$ are the molar flowrate of component i in the inlet and outlet streams to the indoor volume, respectively. The energy balance is given by:

$$\frac{\partial n_{i,b} T_b}{\partial t} = \sum_{j=0}^{inlets} F_{i,j} T_j - \sum_{k=0}^{outlets} F_{i,k} T_k \tag{5}$$

where T_b is the temperature in the indoor volume and T_j and T_k are the temperature of inlet and outlet streams to the

indoor volume, respectively. The component mass balance is given by:

$$\frac{\partial n_{i,b} y_{i,b}}{\partial t} = \sum_{j=0}^{\text{inlets}} F_{i,j} y_{i,j} - \sum_{k=0}^{\text{outlets}} F_{i,k} y_{i,k} \quad (6)$$

where $y_{i,b}$ is the molar fraction of component i in the indoor volume and $y_{i,j}$ and $y_{i,k}$ are the molar fraction of component i in the inlet and outlet streams to the indoor volume, respectively. Since the adsorption isotherms and the pressure drop require the pressure conditions, we should also use the ideal gas equation:

$$y_{i,b} P_b V_b = n_{i,b} R T_b \quad (7)$$

where R is ideal gas constant and P_b is the total pressure in the indoor volume. These equations allow the calculation of $n_{i,b}$, $y_{i,b}$, T_b and P_b . These values are global variables that will be used for the calculations of the adsorption unit, as well as in the valves and the fan used to force the gas to pass through the fixed bed.

The mathematical model of the adsorption process has been previously used for very different applications and is given by a set of equations describing the mass, energy and momentum transfer in a packed bed [37, 38]. Diffusion is described as a bi-LDF (linear driving force) approach and the transient model is solved in only one spatial (axial) coordinate.

The mass balance in the gas phase is:

$$\begin{aligned} \varepsilon_c \frac{\partial C_i}{\partial t} + \frac{\partial(uC_i)}{\partial z} = \varepsilon_c \frac{\partial}{\partial z} \left(D_{ax} C_T \frac{\partial y_i}{\partial z} \right) \\ - (1 - \varepsilon_c) \frac{a k_{m,i}}{(1 + Bi_i/5)} (C_i - \bar{c}_{p,i}) \end{aligned} \quad (8)$$

where C_i is the gas phase concentration of component i , D_{ax} is the axial dispersion coefficient, u is the superficial velocity, y_i is the molar fraction of component i , $k_{m,i}$ is the film mass transfer resistance, $\bar{c}_{p,i}$ is the averaged concentration in the adsorbent particles, C_T is the total gas concentration, ε_c is the column void fraction, a is the adsorbent specific area and Bi_i is the Biot number.

A bi-disperse model for gas diffusion within the adsorbent is used. The mass balance in the macropores of the adsorbent particle is:

$$\frac{\partial \bar{c}_{p,i}}{\partial t} = \frac{15 D_{p,i}}{r_p^2} \frac{Bi_i/5}{(Bi_i/5 + 1)} (c_i - \bar{c}_{p,i}) - \left(\frac{1 - \varepsilon_p}{\varepsilon_p} \right) \rho_s \frac{\partial \bar{q}_i}{\partial t} \quad (9)$$

where $D_{p,i}$ is the macropore diffusivity, r_p is the pellet radius, ε_p is the pellet void fraction, ρ_s is the solid adsorbent density

and \bar{q}_i is the averaged adsorbed concentration of component i .

The mass balance in the micropores of the adsorbent is given by:

$$\frac{\partial \bar{q}_i}{\partial t} = \frac{15 D_{c,i}}{r_c^2} (q_i^* - \bar{q}_i) \quad (10)$$

where $D_{c,i}$ is the micropore diffusivity, r_c is the crystal or micropore radius and q_i^* is the amount adsorbed of component i in equilibrium with the gas phase.

The Ergun equation is used to describe the pressure drop behavior along the column:

$$\frac{\partial P}{\partial z} = -37.5 \frac{\mu_G (1 - \varepsilon_c)^2}{\varepsilon_c^3 r_p^2} u - 0.875 \frac{\rho_G (1 - \varepsilon_c)}{\varepsilon_c^3 r_p} u \cdot |u| \quad (11)$$

where P is the total pressure, μ_G is the gas viscosity and ρ_G is the density of the gas. If a honeycomb monolith or other ordered structures are used, other type of equations should be used to describe the pressure drop in the system. It should be noted that in systems where a fan or compressor passes the air through a bed, a good description of the pressure drop is very important.

Adsorption is an exothermic process and the energy released when adsorption takes place can contribute to increase the temperature of the adsorbent influencing its capacity to adsorb different components. In this work, different energy balances (for the gas phase, the solid adsorbent and the column wall) are used. The reason for using three different energy balances in a generic model is to be able to provide an accurate description of energy transfer provided that the adsorption process for control of indoor air quality may have very different sizes resulting in different heat transport mechanisms. Additionally, having other adsorbent shapes (honeycomb monoliths for example) may result in differences between the gas and the solid temperatures that should be considered to correctly quantify the amount adsorbed. The energy balance in the gas phase is:

$$\begin{aligned} \varepsilon_c C_T \hat{c}_{v_g} \frac{\partial T_g}{\partial t} = \frac{\partial}{\partial z} \left(\lambda \frac{\partial T_g}{\partial z} \right) - C_T \hat{c}_{p_g} \frac{\partial (u T_g)}{\partial z} \\ + \varepsilon_c R T_g \frac{\partial C_T}{\partial t} - (1 - \varepsilon_c) a h_f (T_g - T_s) \\ - \frac{2 h_w}{r_w} (T_g - T_w) \end{aligned} \quad (12)$$

where T , T_s and T_w symbolize the temperature in the gas phase, adsorbent and column wall, respectively, λ is the heat axial dispersion coefficient, \hat{c}_{p_g} and \hat{c}_{v_g} are the gas molar specific heat at constant pressure and volume, respectively, r_w is the internal radius of the cylindrical column and h_w and

h_f as the film heat transfer coefficient between the gas phase and wall, and between gas phase and adsorbent, respectively. The energy balance in the solid phase is:

$$\left[\varepsilon_P \sum_{i=1}^{nc} (\bar{c}_{p,i} \hat{c}_{Vg}) + \rho_P \sum_{i=1}^{nc} (\bar{q}_i \hat{c}_{Vads}) + \rho_P \hat{c}_{Ps} \right] \frac{\partial T_S}{\partial t} = \left[\varepsilon_P R T_S \sum_{i=1}^{nc} \left(\frac{\partial \bar{c}_{p,i} \hat{c}_{Vg}}{\partial t} \right) + ah_f (T_g - T_S) \right] + \frac{\rho_P}{(1 - \varepsilon_C)} \sum_{i=1}^{nc} \left(-\Delta H_i \frac{\partial \bar{q}_i}{\partial t} \right) \tag{13}$$

where \hat{c}_{Vads} is the molar specific heat at constant volume of adsorbed, \hat{c}_{Ps} is the heat capacity coefficient of the material used to build the packed bed column and ΔH_i is the heat of adsorption of component i . The energy balance of the column is given by:

$$\rho_w \hat{c}_{pw} \frac{\partial T_w}{\partial t} = \frac{d_w}{e(d_w + e)} h_w (T - T_w) - \frac{U}{(d_w + e) \ln \left(\frac{d_w + e}{d_w} \right)} (T_w - T_\infty) \tag{14}$$

where \hat{c}_{pw} is the specific heat of the column wall, U is the heat transfer coefficient to the external environment with a temperature T_∞ , ρ_w is the density of the material of the column wall, d_w is the column diameter and e is the thickness of the column wall.

The valves used in the system to communicate the different streams have simple open and close commands and the equation to describe them is:

$$F_{out} = S_p X_v \Delta P \tag{15}$$

where F_{out} is the volumetric flowrate at the exit of the valve, S_p is the stem position defined as 1 for an open valve and 0 for a closed valve, X_v is the flow coefficient of the valve and ΔP is the pressure difference between inlet and outlet of the valve.

Since the compressor / fan used for the system depends strongly on the size and type of gases, in this initial work, a simple pressure driven flow was used where the pressure outlet (P_{out}) is calculated by:

$$P_{out} = G_f P_{in} \tag{16}$$

where P_{in} is the inlet pressure and G_f is the pressure gain coefficient.

To this set of equations, a system inlet and outlet were added to account for possible mass transfer coming and exiting the system, but that may not apply in all cases. The mathematical model of the system was solved in gPROMS (PSE Enterprise, UK). The equations in the adsorption column were solved with the orthogonal collocation of finite elements (OCFEM). A screenshot of the topology

implemented in gPROMS is shown in the Supplementary Information together with the parameters needed to make the simulations for the two case studies presented in this work.

3 Results and discussion

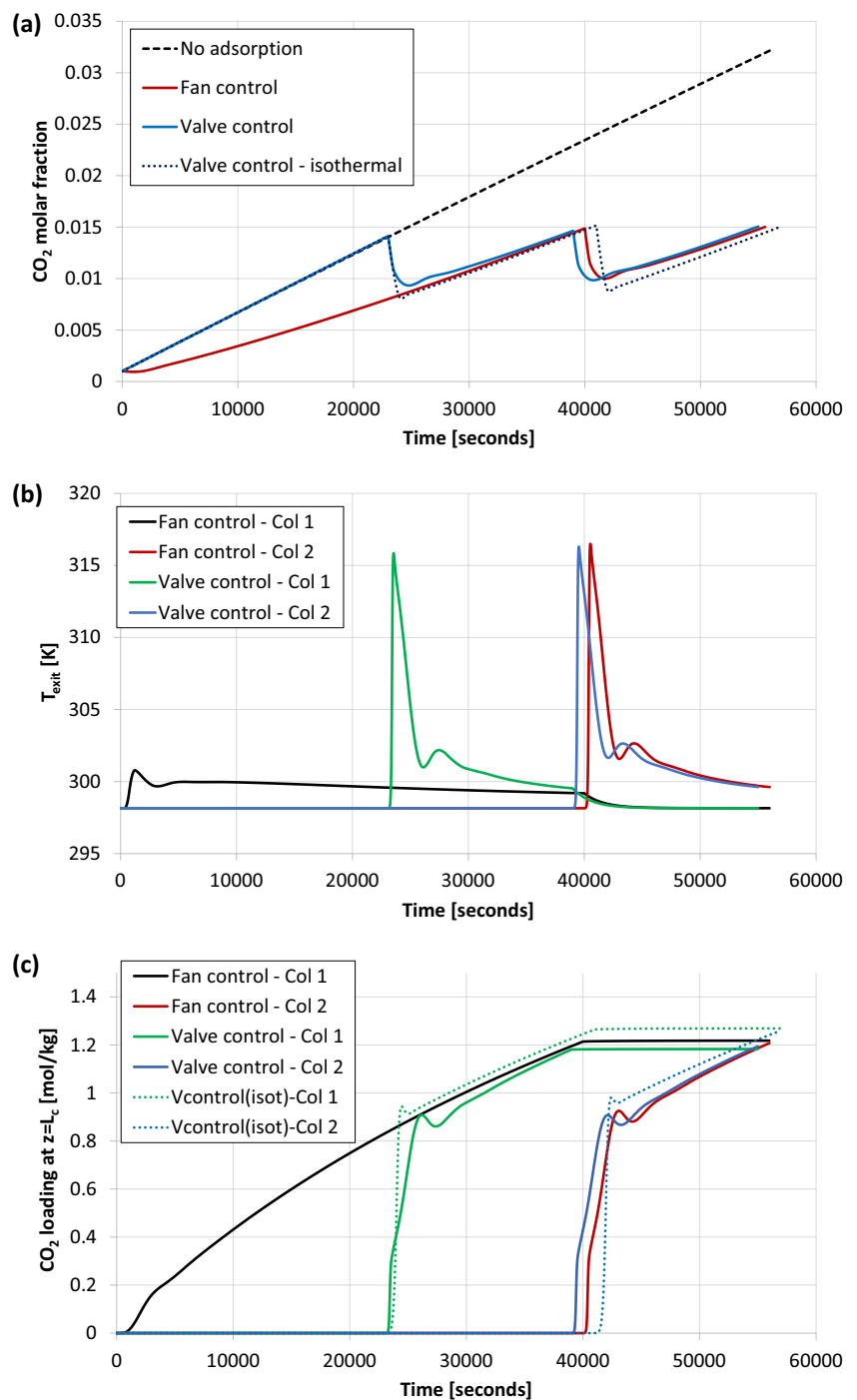
3.1 First example: continuous CO₂ removal from closed environments

In closed environments (like spaceships or submarines) where the air cannot be recycled, accumulation of carbon dioxide from respiration occurs. From an adsorption technology perspective, a higher concentration of CO₂ results in higher loading in the adsorbent and thus a smaller size is required. However, since high CO₂ concentration affects the health of the crew, a compromise should be found. While the international space station has a volume of approximately 1000 cubic meters for a crew of seven astronauts, other spaceships where CO₂ removal technology is required, have a more compact design. For this work, the volume of gas to be treated was assumed to be 25 cubic meters for a crew of 2 astronauts. The two adsorption columns have a column radius and length of 0.15 m and are filled with zeolite 13X [39]. The rest of the details used in the simulations are listed in the Supplementary Information. Since this work only aims to demonstrate the modeling approach, water effects were not considered in the simulations. Indeed, for an improved CO₂ removal under humid conditions, other type of materials can be used, like activated alumina [40] or some amine-loaded materials.

The molar fraction of CO₂ in the closed volume is shown in Fig. 2a for the initial hours of operation (using two adsorption columns). The first result is obtained assuming that there is no CO₂ cleaning technology. If no air treatment is applied, after 15 h (54,000 s), the amount of CO₂ increases linearly to over 3% which is dangerous for the health of the astronauts.

The CO₂-removal technology employed can be operated in several ways. One possible operation method is that the unit is controlled by opening and closing valves while the fans are all time operating (termed here as valve control) so the gas is passing all time through one column. The columns are shifted when a certain gas molar fraction is obtained at the exit of the feed-processing column. The result of this approach leads to an initial longer utilization of the first column because the adsorbent starts adsorbing sequentially CO₂ from low concentrations and heat effects are minimized. In this example, a CO₂ molar fraction of 1.5% in the indoor (batch) volume was established as an arbitrary limit. It can be observed that the first column can process the air for 40,000 s while the CO₂ concentration is

Fig. 2 Effect of process operation in controlling the amount of CO₂ in a closed environment: **a** molar fraction of CO₂ in the volume to be purified; **b** temperature profile at the end ($L_c=0.15$ m) of the adsorption processes and **c** amount of CO₂ adsorbed at $L_c=0.15$ m for each column



building up in the indoor (batch) volume. In cyclic operation where CO₂ is already built up in the indoor volume, the adsorption column performance will be closer to the one observed with the second column, that can process air for 16,000 s.

Alternatively, the technology can be started by turning on the compressors or fans only when the target molar fraction is achieved (termed here as fan control). This

means that the initial period (23,000 s for this example), the gas will not be passing through the adsorption columns and it will only start passing through when 1.5% CO₂ is detected in the indoor (batch) volume.

When these results are plotted in the same graphic, it is possible to see that there are clear differences between these two approaches, caused only by having a different initialization procedure. When the air can pass through the first column

from the initial moments when the contaminant concentration is very small, the temperature increase of the adsorbent bed is also very small since there is enough time to dissipate the heat generated. On the other side, when the gas enters the column already having 1.5% CO₂, there is a faster adsorption that results in a stronger thermal increase of almost 20 K. The temperature at the exit of the adsorption columns for the cases described in this section are plotted in Fig. 2b. In the locations where the temperature increases, the local capacity of the adsorbent is smaller. Since the column cannot evacuate the heat fast enough, the adsorbent remains warmer for a longer period of time resulting in a net lower adsorption capacity. This is one of the reasons why the energy balance should be solved together with the mass balance; if the mathematical modelling considered the operation as isothermal, a better performance (longer column operation) could have been obtained as shown in Fig. 2a.

In Fig. 2c the amount of CO₂ adsorbed at the end of the column is shown. As a consequence of the temperature oscillation, an initial peak is obtained in the analyzed cases. It should also be noted that once that the feed concentration of CO₂ is changing at all time, the CO₂ "plateau" normally obtained in breakthrough curves will not occur because of continuous generation. In that regard, when the molar fraction is around 1.5% the adsorbent has a capacity to adsorb around 1.2 mol/kg of CO₂. However, as the concentration decreases, the capacity also decreases and this is the reason for the first initial peak observed, both in the temperature and in the amount adsorbed.

In designing adsorption processes for air quality control, the standard approach is to use a fixed bed concentration and then "size" the unit. Integrating the adsorption process with the indoor volume allows an accurate sizing of the adsorption unit, but it can also help with having a more adapted process control because tailored sensors can be placed in the volume to be controlled. With the standard approach, the concentration changes within a given indoor (batch) volume are not considered and as can be seen from the results, the concentration of the component will be oscillating between the target value and one lower value that is proportional to the amount of CO₂ adsorbed, to its diffusional resistances and also to the thermal management of the separation unit.

3.2 Second example: peak shaving of water in bathrooms

Another application where adsorption processes can have a significant impact in indoor quality control is to remove concentration peaks of a given contaminant or component. Common examples are VOCs after painting and water removal from a bathroom after a shower. Although water cannot be directly considered as a contaminant, it promotes the formation of mold in the more stagnant zones of the bathroom requiring periodic cleaning and repainting. The

need for a dehumidifier strongly depends on the weather and housing temperature conditioning [41]. Commercial dehumidifiers do exist, but a technology based on adsorption can be less noisy, more compact and energy efficient. In places with mild temperatures and poor (or expensive) heating, the temperature of the bathroom can be 16–18 °C in winter at the moment to start the bath / shower. Depending on the design of the bathroom and the shower box, a shower with water at 37 °C will result in a sudden increase of the relative humidity of the bathroom from somewhere within the comfort zone (35–65% relative humidity) to saturation. Longer shower time will also result in condensation of water in the bathroom walls and ceiling.

As an example, it is assumed that the bathroom volume is 10 cubic meters and an initial temperature of 291 K (18 °C). The relative humidity at the beginning of the shower is fixed at 50%. When the humidity in the bathroom achieves 70% (outside of the comfort zone), the adsorption unit starts operating. The shower lasts for 7 min and then generation of water vapour ceases, but the adsorption process keeps operating to return the humidity to the comfort zone (below 65% with a target in 50%). In this work, the focus is only to see what happens in the bathroom and the regeneration of the material will not be studied.

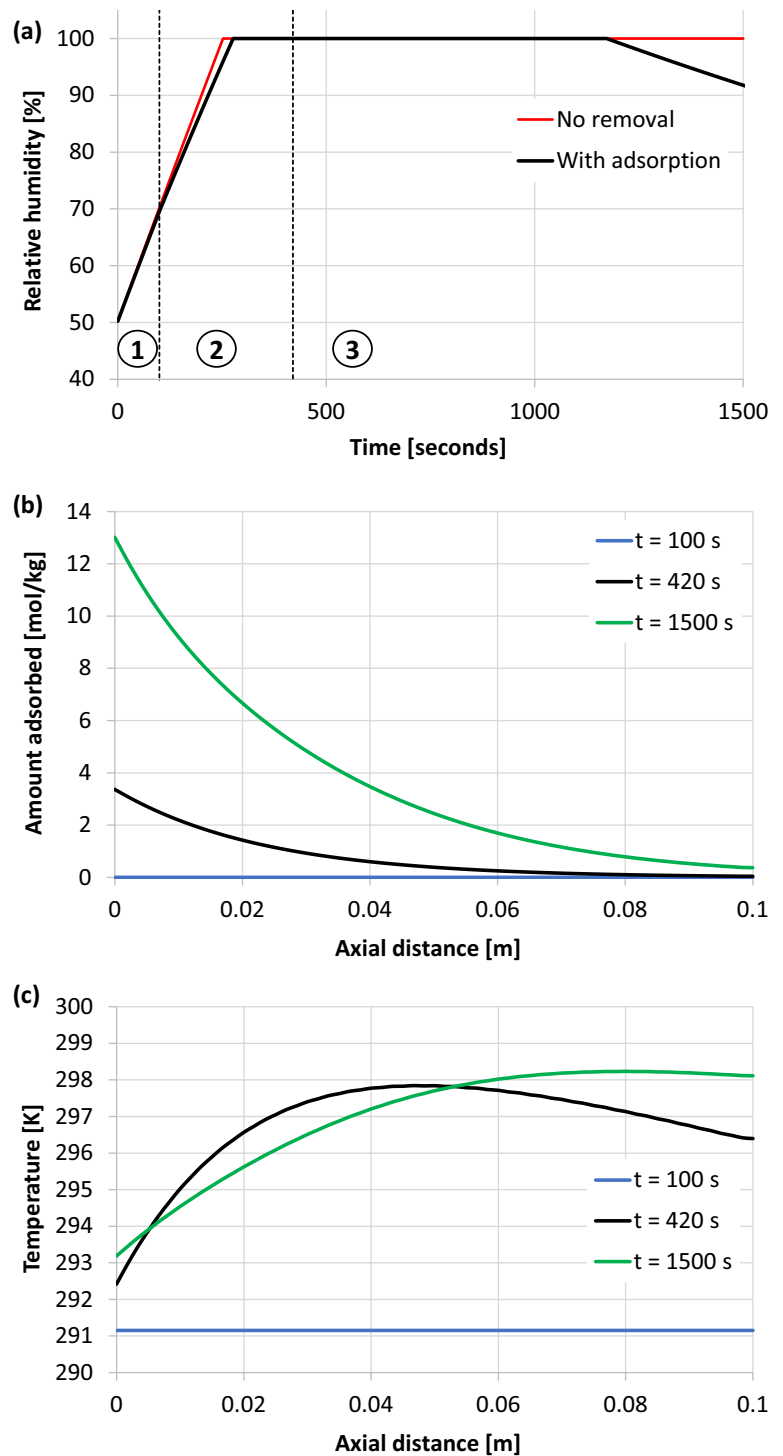
For this initial work, a bed of silica gel (cheap adsorbent) was used and the properties of the material, adsorption isotherms and diffusional parameters are available in literature [42]. This example shows how the sizing of the equipment can be tuned for a more efficient water removal from this specific bathroom volume.

Without any water removal technology in the bathroom, the relative humidity attains 100% after 250 s (4.2 min), assuming a rate of water vapor generation of 23 L per minute at 310 K. After reaching 100% relative humidity and before water generation finished, liquid water will start condensing in colder surfaces (walls, ceiling, mirrors, etc.). The amount of water that enters the bathroom is 6.3 mol and assuming a silica gel capacity of 10 mol/kg, around 630 g of adsorbent will be needed to remove the entered amount of water. The adsorption equilibrium of water at 50% RH (at 291 K) is approx. 15 mol/kg, so assuming a loading of 10 mol/kg should compensate for losses in overall column capacity due to axial dispersion, diffusion and thermal effects.

In Fig. 3, the relative humidity of the bathroom is shown for the base case where no water removal technology is used and for the case when a unit containing 630 g of silica gel is used. The length of the column is $L=0.1$ m and the porosity is $\epsilon_c=0.4$ (the rest of the values used for the simulations are reported in the Supplementary Information).

The adsorption technology only starts working when the relative humidity of the bathroom reaches 70% (step 1 in Fig. 3 while the water generation lasts until the end of step 2). As can be seen in Fig. 3, it takes a very long

Fig. 3 **a** Relative humidity in the indoor volume with and without water removal, **b** amount adsorbed along the bed at three different times and **c** temperature along the bed at three different times



time until the relative humidity is controlled using this unit design. The amount of silica used efficiently is rather small and the main reasons are: (a) temperature increase due to adsorption, (b) rather low velocity through the bed and (c) diffusional effects. Increasing the gas velocity in the bed while keeping the same bed dimensions will result in additional power consumption and noise, which is not desired.

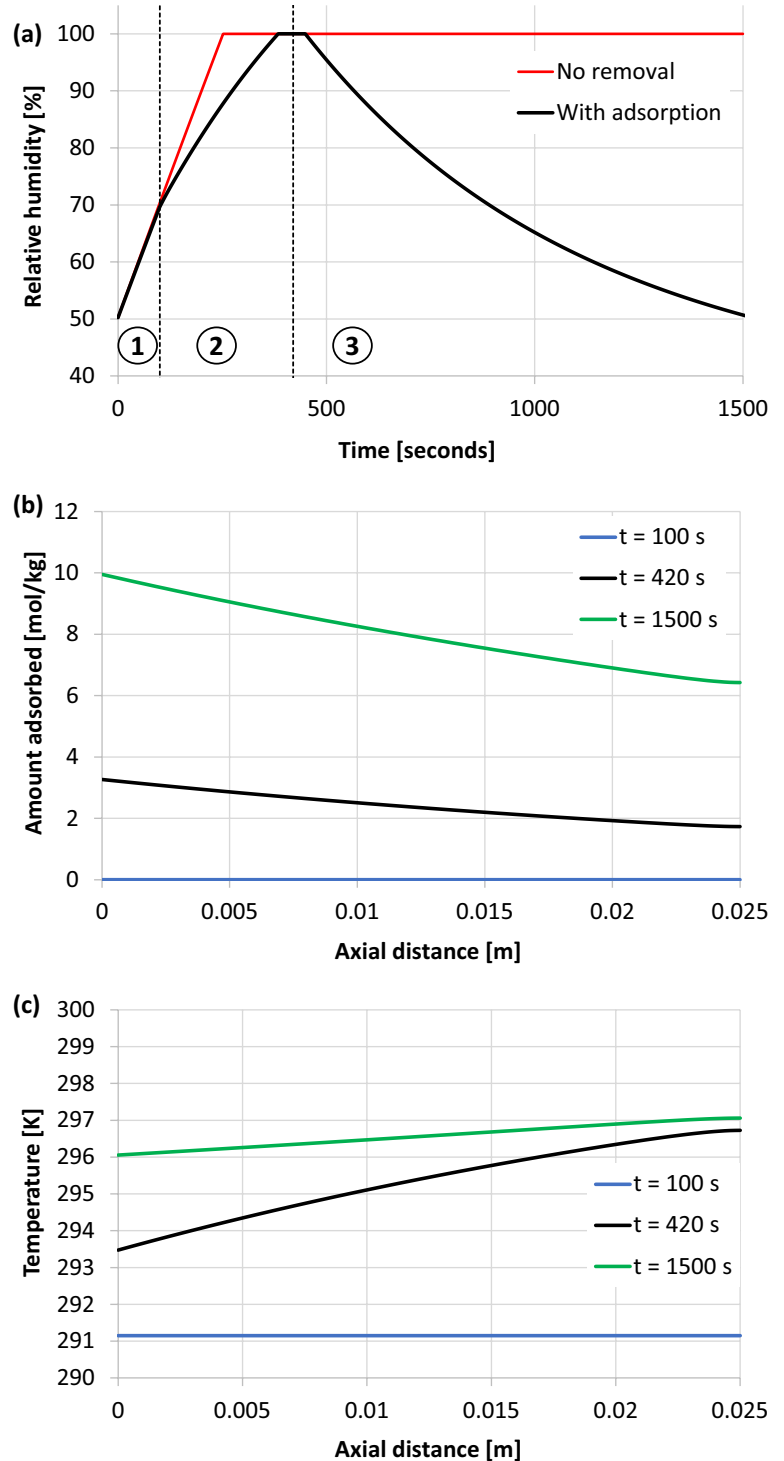
The thermal effects can only be reduced by adding some elements with higher heat capacity to the column [43].

Since the gas velocity through the adsorption unit is driven by pressure drop, a possibility to increase the gas velocity is to distribute the adsorbent in a shorter and thicker column [44]. If the column length is decreased by half and

the radius of the column is increased by a factor of $\sqrt{2}$, the gas velocity can be increased from 0.23 m/s to 0.34 m/s. The results of this simulation are shown in the Supplementary Information. Although the performance of the unit is significantly better, there is still condensation of water for a significant period and reestablishing the relative humidity

at 50% takes long time. For this reason, a further reduction in the bed length to 0.025 m (doubling the original column radius to 0.099 m) results in an increase in gas velocity to 0.40 m/s. The results of this simulation are shown in Fig. 4. Only by changing the column dimensions it is possible to make a much better adsorbent utilization. Although there is still a period where condensation is observed, this period

Fig. 4 **a** Relative humidity in the indoor volume with and without water removal with $L_c/R_c=0.25$, **b** amount adsorbed along the bed at three different times and **c** temperature along the bed at three different times



is very small and the relative humidity of the bathroom is reestablished after 20 min of operation. One of the important differences is that the temperature of the column is reduced because more gas enters the column and can contribute to cool down the adsorbent.

It has been shown that having a mathematical model with a good system description can help in improving the adsorbent utilization by changing the shape of the column. The design with a $L_c/R_c = 2$ used initially results in a high pressure drop that limits the gas velocity inside the column and thus the column cannot be cooled down fast enough. The design with a $L_c/R_c = 0.25$ ratio results in a faster adsorbent cooling promoted by a high gas velocity. A system with a radial feed is perhaps a more efficient and compact manner to implement low L_c/R_c ratios. A process design that renders smaller beds should be favored. Such beds can be regenerated faster and at the same time can reduce capital cost. However, the size reduction will ultimately be defined by parameters like diffusion and dispersion and eventually thermal effects.

From the process point of view, another option that can be evaluated is how the shaping of the adsorbent impacts

the process [45, 46]. This evaluation starts by assuming that the properties of the adsorbent will be rather independent of the shaping (that should be verified experimentally). In the examples shown before, the diffusional limitations in the silica particles with a diameter of 2 mm are important, affecting the performance of the system. Decreasing the particle diameter to reduce diffusional resistances, will result in a larger pressure drop, so a tradeoff situation should be found. Although with this detailed model is also possible to find such tradeoff, the objective of this publication is only to demonstrate the features of a tailored model. The performance of the unit using particles with a diameter of 1 mm changes significantly as shown in Fig. 5. With smaller particles, the benefits of reduced diffusional limitations are more important than the loss of inlet gas velocity due to a larger pressure drop. The faster initial adsorption also results in a larger temperature excursion at the beginning of the operation, but the short length of the column contributes to a faster and efficient cooling. The cooling is not as efficient as in the results with the bigger particles (shown in Fig. 4) because the gas velocity is smaller. Indeed, it is observed

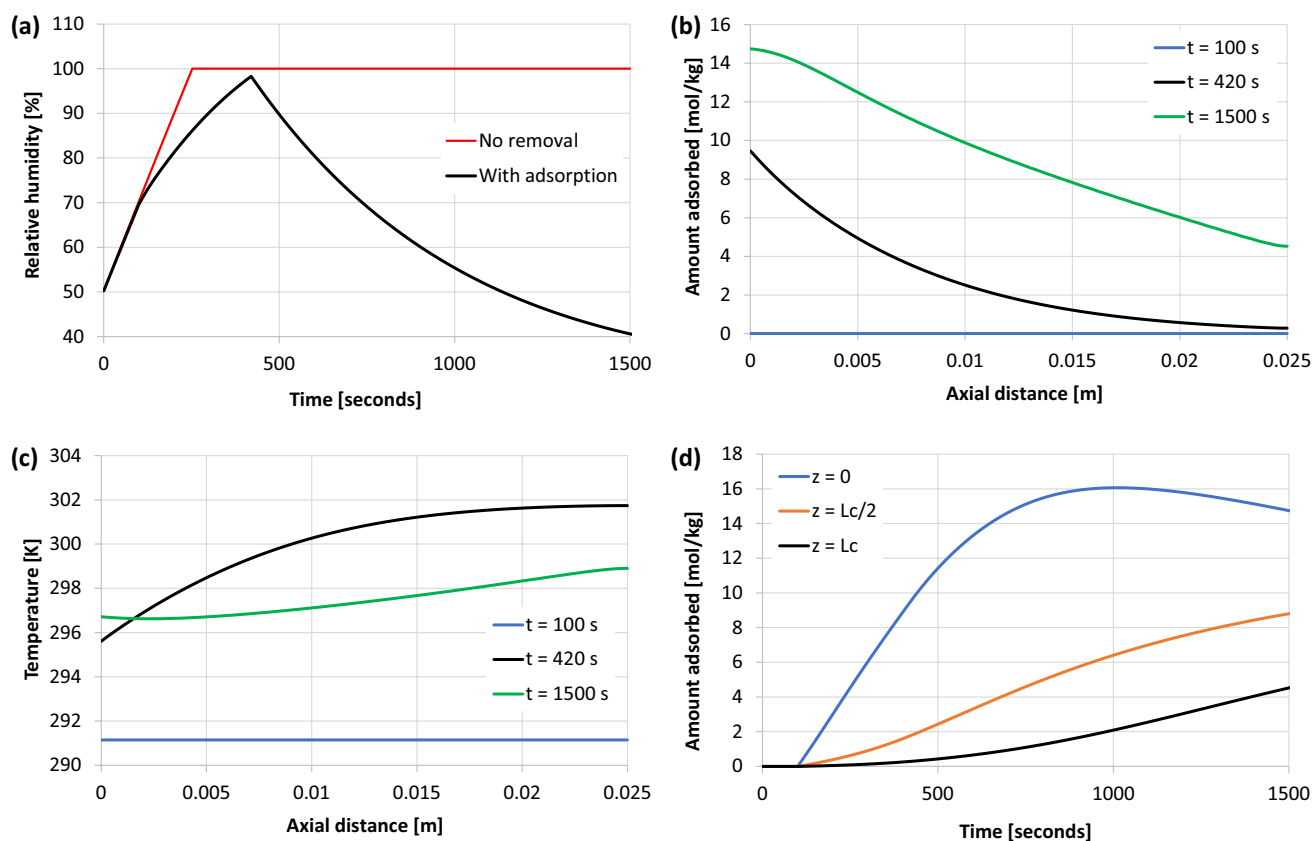


Fig. 5 **a** Relative humidity in the indoor volume with and without water removal with $L_c/R_c = 0.25$ and silica particles with 1 mm diameter, **b** amount adsorbed along the bed at three different times, **c** tem-

perature along the bed at three different times and **d** evolution of the amount adsorbed in three different positions of the column

that tailoring the adsorbent shape can be part of the strategy to achieve full process performance.

There are also two important things that should be mentioned. Controlling the process performance with the relative humidity can be slightly misleading when the temperature of the gas in the room changes. In Fig. 5, the operation for longer periods can take the relative humidity to values lower than the initial ones. However, the molar fraction in the gas phase only returns to the original place. The difference is in the saturation pressure because the temperature of the gas in the bathroom increases by almost 5 K degrees. Another important aspect shown in Fig. 5 is the evolution of the amount of water adsorbed in different positions of the column. If the system was modelled and designed with a constant water relative humidity of 50%, the amount adsorbed of water could not exceed 15 mol/kg. The higher capacity of the adsorbent in the period where the amount of water vapor is between 50–100% relative humidity is retained and that is why a more accurate description of the equipment can be obtained.

3.3 Future possibilities for adsorption technologies in IAQ markets

In many countries, indoor air should comply regulated standards, at least in commercial and industrial buildings. Digitalization and advanced automation of diverse equipment are bringing advanced control of technologies to new platforms. Adsorption technologies have all possible advantages to be integrated into complex multi-purpose cleaning units with centralized control [47]. As mentioned before and as practiced in other adsorption applications, layering materials can be used to remove multiple components and this can be a factor for economical design of units in larger commercial buildings.

Large variety of materials has been reported in the last years; the metal–organic framework (MOF) community has a very powerful toolbox to tailor-design materials for different applications. Such utilization for advanced and miniaturized sensors that allow fast and reliable detection can be very powerful for advanced IAQ equipment control.

On a side note, it should be mentioned that the removal of any particular contaminants from commercial buildings is achieved by permanent air circulation. On the other side, the presence of human beings grants that the CO₂ concentration in that air will be higher than in outdoor environments. Considering these factors (granted forced movement of air and higher CO₂ concentration), CO₂ capture from indoor environments should be more energy-efficient than CO₂ capture from outdoors. Rotating wheel process was already suggested for CO₂ removal from rather diluted flue gas streams and imposing a low pressure drop [48].

It is still unknown how will be the implementation of new IAQ technologies in a pos-pandemic scenario with remote working and enhanced online shopping of items. Although this should not affect the design of the technologies, this market context can drive the technological development towards residential applications, where adsorption can have benefits over other technologies.

4 Conclusions

This work presents a generic model of a packed bed adsorption process integrated in a finite volume representing an indoor volume where the concentration of a particular species (contaminant) should be controlled. The mathematical model of the system is used for two different examples of application: continuous removal of CO₂ from closed environments and removal of peaks of water from bathrooms. The results obtained indicates that even for removal of small concentration of gases, the thermal effects can be important for designing these systems. Moreover, when the adsorption technology is driven by a fan and the flow of gas is regulated by the pressure drop along the column, the mathematical model can assist in achieving a good L_c/R_c ratio that optimizes performance. Finally, it was also shown that assuming that the properties of the material are not changing with its shape, this mathematical model can also provide indications of the adequate shaping where a tradeoff between pressure drop and diffusion and/or thermal effects is achieved.

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