Mekanika: Majalah Ilmiah Mekanika

Adsorption Characteristics of Silica Gel-Water Pairs in Personal Protection Equipment

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Abstract
This study aims to determine the characteristics of silica gel RD to water vapor in terms of adsorption capacity and rate. A layer modeling approach was employed to simulate the Personal Protective Equipment (PPE), which comprised four distinct layers: the surrounding environment air, the fabric layer, the RD-type silica gel layer, and the air gap separating the silica gel from the skin surface. The simulation encompassed environmental conditions set at 27 ℃, while the human body's temperature was maintained at 35 ℃. This study uses a simulation method using Guggenheim–Anderson–de Boer (GAB) modeling calculations to determine isothermal characteristics and Linear Driving Force (LDF) modeling to determine kinetic characteristics with an adsorbent temperature of 26.84 ℃. The simulation results show that the isothermal characteristics of silica gel RD at a relative humidity of 60% or a relative pressure of 0.6 have an absorption capacity of 0.38 kg/kg. Moreover, the kinetic characteristics of silica gel RD have an absorption rate of 0.38 kg/kg of water vapor with a time of 980 s until a significant reduction in the absorption value occurs.

1 Introduction

Field workers, especially health workers, must use Personal Protective Equipment (PPE) when working or performing their duties. PPE serves to maintain the safety and security of workers in a hazardous work environment. According to World Health Organization (WHO), in the current era of the Coronavirus Disease 2019 (COVID-19) pandemic, especially for health workers are required to use PPE in the form of medical masks, goggles, face masks, gloves, and especially hazmat clothes to prevent the spread of COVID-19. Certain ergonomic requirements must be met when using PPE to reduce discomfort caused by physiological or mental stress factors of health workers. Researchers have developed and innovated international standards for determining the protection factors for various types of PPE [1].

PPE improvisation is needed to prevent heat stress. Heat stress is a condition where the body can no longer maintain the body temperature. In tropical climates, which have an environmental temperature of 25-34 °C to prevent heat stress, PPE, which can limit the evaporation of excess heat, is needed [2]. PPE is

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generally made of thick, multi-layered, and heavy material. This material causes thermal circulation to be hampered because it reduces the rate of heat exchange and the limited water vapor permeability of the clothing layer. The result is an increase in temperature inside the PPE, which can become a significant issue, especially in hot conditions or when working in hazardous environments. It not only diminishes user comfort but can also be harmful to their health [2].

The equipment that uses PPE must have guaranteed safety and quality, but comfort must still be considered by ensuring that these materials remain comfortable to use on the human body. To achieve thermal comfort and maintain the body temperature at 37 °C, the layers of PPE material need to be combined with other adsorbent materials, such as silica gel [3]. This addition plays a crucial role in enhancing the overall user experience. Within the realm of PPE, maintaining the appropriate moisture level is the key to user comfort and health. Silica gel functions as an effective moisture-absorbing agent, capturing moisture that may accumulate within PPE during use. Silica gel has characteristics that are very suitable for adsorption, namely providing a cooling effect for water with a low heat source or below 85 °C [4].

Over a wide range of pressures, the isotherm characteristics of silica gel in relation to water vapor can be observed. At low pressures, silica gel has a low adsorption capacity for water vapor. RD-type silica gel can achieve 95% regeneration at 90 °C, and at 140 °C, it can desorb 95% in four minutes and has a high cooling capacity [5-7]. Research becomes highly significant as it can provide valuable insights into the isotherm and kinetic properties of RD-type silica gel when used as an adsorbent in Personal Protective Equipment (PPE). Furthermore, the objective of this research is to assess the impact of using silica gel in PPE materials to improve user comfort.

Silica gel-water, also known as silica gel, is a popular material in Personal Protective Equipment (PPE) due to its desiccation capability, low humidity, protection against rust and corrosion, and ability to reduce mold and mildew growth [8]. It can be regenerated easily, making it a cost-effective solution for PPE. Aqueous silica gel is compatible with various PPE materials, making it a versatile choice for various types of personal protection [9,10]. It is non-toxic but should not be consumed, making it safe for use in PPE and work environments [11]. However, proper usage and careful manufacturer instructions are essential to maintain its effectiveness [12,13].

2 Experimental Methods

2.1 Heat transfer

Figure 1 illustrates the layers used in the modeling process for this study. The layer modeling comprises the skin surface, an air gap, silica gel, fabric, and the surrounding environment. The analysis of heat and mass transfer resulting from the introduction of silica gel to Air-Purifying Respirator (APD) was conducted utilizing the Nusselt number (*Nu*) and Linear Driving Force (LDF) functions to compute the adsorption rate. Additionally, the Guggenheim–Anderson–de Boer (GAB) model was employed to calculate the adsorption rate. The analysis of heat and mass transfer encompasses the properties of air, fabric, silica gel, and the skin.

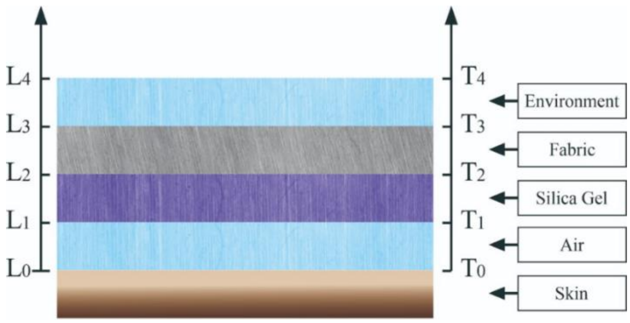

Figure 1. Layer modelling

The following Equation calculates heat transfer and mass transfer in layers. According to the law of energy balance, heat transfer is calculated by taking the thermal resistance for convection and conduction into account. The mass transfer involves the mass resistance of the silica gel and cloth, as shown in Equations 1-4 [14,15].

$T_0 - T_1$

$$Q_{air} = h_1 A_1 (T_0 - T_1) = \frac{1}{R_{conv,1}} (T_0 - T_1) \tag{1}$$

$T_1 - T_2$

$$Q_{silicagel} = \frac{k_2 A_2 (T_1 - T_2)}{L} + \Delta H_{ads} k_{m,2} A_2 (X_1 - X_2)$$
$$= \frac{1}{R_{cond,2}} (T_1 - T_2) + M_{v,2} \Delta H_{ads} \tag{2}$$

$T_2 - T_3$

$$Q_{fabric} = \frac{k_3 A_3 (T_2 - T_3)}{L} + \Delta H_{ads} k_{m,3} A_3 (X_2 - X_3)$$
$$= \frac{1}{R_{cond,3}} (T_2 - T_3) + M_{v,3} \Delta H_{ads} \tag{3}$$

$T_3 - T_4$

$$Q_{environment} = h_4 A_4 (T_3 - T_4) = \frac{1}{R_{conv,4}} (T_3 - T_4) \tag{4}$$

2.2 Isotherm modelling

The isothermal adsorption characteristics were obtained using GAB modeling to get the equilibrium adsorption uptake (*q*) value as in Equations 5-8, which are used to find the constant variable related to heat [16].

$$w_{eq} = \frac{w_m CK(P/P_0)}{[(1 - K(P/P_0)][(1 - K(P/P_0) + CK(P/P_0)]} \tag{5}$$

$$w_m = w_{mo} exp \frac{q_m}{RT_{ads}} \tag{6}$$

$$C = C_o exp \frac{\Delta H_c}{RT_{ads}} \tag{7}$$

$$K = K_o exp \frac{\Delta H_k}{RT_{ads}} \tag{8}$$

Where P is the pressure, P_0 is the saturation pressure, and R is the specific gas constant for water vapor; w_{mo}, q_m, K, C, K_o, and C_o are variable constants related to the heat; ΔH_c, ΔH_k are the water vapor sorption heats.

2.3 Kinetic modelling

The Linear Driving Force (LDF) model is the most commonly used model to calculate adsorption kinetic. The adsorption rate (*dw\dt*) can be calculated in terms of the adsorbent/adsorbate pair by Equations

9-13 [17]. The Arrhenius equation in Equation 14 [18] can be used to obtain the D_s parameter, namely the diffusion coefficient on the surface. According to the journal references, Equation 15 can be used calculate k_m, the total mass transfer coefficient given in Equation 15, where the value of F_0 is 15.

$$\left(\frac{dw}{dt}\right) = \frac{F_0 D_s}{R_p^2}\left(w_{eq} - w(t)\right) \tag{9}$$

$$F = 1 - \exp(-F_0\theta) \tag{10}$$

$$F = \frac{w(t) - w(0)}{w_{eq} - w(0)} \tag{11}$$

$$\theta = \frac{D_s}{R_p^2} t \tag{12}$$

$$\ln(1 - F) = -F_0\theta = -F_0 \frac{D_s}{R_p^2} t \tag{13}$$

$$D_s = D_{so} exp \frac{-E_a}{RT_{ads}} \tag{14}$$

$$k_m = F_0 \frac{D_s}{R_p^2} = \frac{15 D_s}{R_p^2} \tag{15}$$

2.4 Properties

Table 1. shows the values of the variables listed in Equations 1-15 and used to solve these equations.

Table 1. Properties for Equations 1-15

Properties	Symbol	Value	Unit
Relative humidity	φ	60	%
Skin temperature	T_0	35	℃
Air temperature	T_1	27	℃
Air surface area	A_1	4	m^2
Layer thickness	L	3×10^{-4}, 1×10^{-3}	m
Layer length	P	5×10^{-4}	m
Humidity ratio of air	X_1	0.018	–
Silica gel mass transfer coefficient	k_{m2}	0.32	$kg/m^2\ s$
Silica gel area	A_2	4	m^2
Silica gel temperature	$T_{2/ads}$	26.84; 26.45	℃
Humidity ratio of silica gel	X_2	0.017	–
Thermal conductivity of silica gel	k_2	0.198	$W/_{m \cdot K}$
Heat of adsorption	ΔH_{ads}	2500	$kJ/_{kg}$
Fabric temperature	T_3	26.643; 25.77	℃
Fabric surface area	A_3	4	m^2
Overall mass transfer coefficient	k_m	2.66×10^{-3}	$kg/m^2\ s$

Table 1. *Cont.*

Properties	Symbol	Value	Unit
GAB isotherm model parameters	w_m	0.361	$kg/_{kg}$
	w_{mo}	0.04	$kg/_{kg}$
	C	4.4343	$-$
	K	0.46	$-$
	C_o	0.4	$kg/_{kg}^{-1}$
	K_o	7.3×10^{-13}	Pa^{-1}
	q_m	0.45	$kJ/_{kg}$
Functions related to heat adsorption	ΔH_c	336.394	$kJ/_{kg}$
Functions related to heat adsorption	ΔH_k	2833.249	$kJ/_{kg}$
Constant gas	R	0.4615	$kJ/_{kg \cdot K}$
Relative pressure	P/P_0	$0 - 0.9$	$-$
Geometry parameter	F_0	15	$-$
Surface diffusivity	D_s	8.392×10^{-12}	$m^2/_s$
Pre-exponential coefficient	D_{so}	24×10^{-4}	$m^2/_s$
Activation energy	E_a	4.2×10^4	$kJ/_{kg}$
Radius of adsorbent particles	R_p	1.74×10^{-4}	m

3 Results and Discussion

3.1 Isothermal adsorption

This study conducted a simulation to collect data in the form of isothermal adsorption characteristics in the silica gel adsorption process with water vapor. The data obtained from the simulation are utilized to determine the equilibrium absorption performance of the adsorption process on silica gel adsorbents against water vapor. Isothermal adsorption simulations were carried out using the GAB modeling equation. The temperature used in the simulation was 26.84 °C, with a predetermined relative pressure range of 0.1 to 0.9.

In this simulation, this temperature condition was employed to represent various potential scenarios, and different relative pressure levels was used to understand how adsorption occurs at varying relative humidity levels. The results of this simulation are crucial for understanding how silica gel behaves when interacting with water vapor under various conditions, which can be valuable in practical applications and gaining a deeper understanding of the adsorption process.

Figure 2 compares the equilibrium adsorption uptake (w_{eq}) value or the equilibrium absorption performance value of the adsorption process with a predetermined relative pressure. Figure 2 shows a significant increase in the value of (w_{eq}), often with an increase in the relative pressure value. These simulation results align with the theory of isothermal adsorption, where it is evident that the more significant the relative pressure value, the greater the equilibrium adsorption uptake. In this context, this finding confirms the fundamental principles associated with isothermal adsorption, implying that with an increase in relative pressure, the adsorbent material's ability, in this case, silica gel, to attract and retain water vapor molecules also increases.

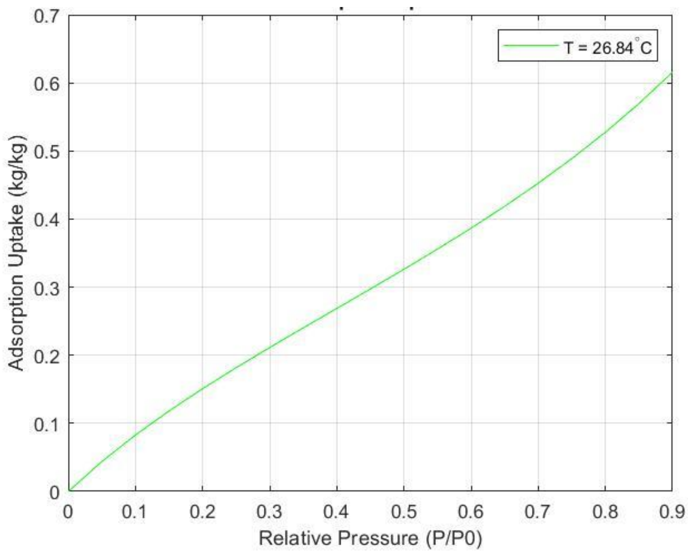

Figure 2. Adsorption uptake isotherm

The isothermal characteristic of the adsorption process reveals the remarkable capabilities of the RD-type silica gel adsorbent. Its ability to absorb water vapor under varying relative pressure and humidity conditions is demonstrated. At a relatively low relative pressure of 0.1, equivalent to a 10% relative humidity, the adsorbent efficiently absorbs 0.0439 kg of water vapor per kilogram of its mass, showcasing its effectiveness even in low humidity conditions. However, as the relative pressure steadily rises to 0.9, corresponding to a high 90% relative humidity, the adsorbent's performance escalates significantly, with a water vapor absorption capacity of 0.6158 kg/kg, highlighting its efficiency in high humidity environments.

In this study, a relative humidity of 60%, equivalent to a relative pressure of 0.6, was selected for testing. The RD-type silica gel adsorbent demonstrated its ability to absorb 0.3867 kg of water vapor per kilogram of its mass under these conditions, underscoring its versatility and effectiveness in various practical applications, particularly in environmental humidity control systems. Understanding these isothermal characteristics provides valuable insights for engineering and industrial applications, where silica gel adsorbents play a crucial role in moisture management.

3.2 Kinetic adsorption

The adsorption kinetic simulation was conducted utilizing the LDF modeling equation. The simulation employed a temperature of 26.84 °C, with a predefined time range spanning from 0 to 3000 seconds and a constant gas input (R) of 8.134 J/mol. The equilibrium adsorption uptake value, which serves as the reference point, was established at a relative pressure of 0.6 or under ambient conditions with a relative humidity of 60%. This comprehensive approach enabled a detailed analysis of the adsorption kinetics of the RD–type silica gel adsorbent under specific environmental conditions, providing valuable insights into its performance over time and improving our understanding of its practical applications in various settings.

Figure 3 compares the instant adsorption value (w) or the instant absorption performance value of the adsorption process with a predetermined time. Figure 3 depicts an increase in value as time is added to the achievement value. The simulation results are in accordance with the adsorption kinetic, in which the adsorption value increases rapidly with time until it reaches the points.

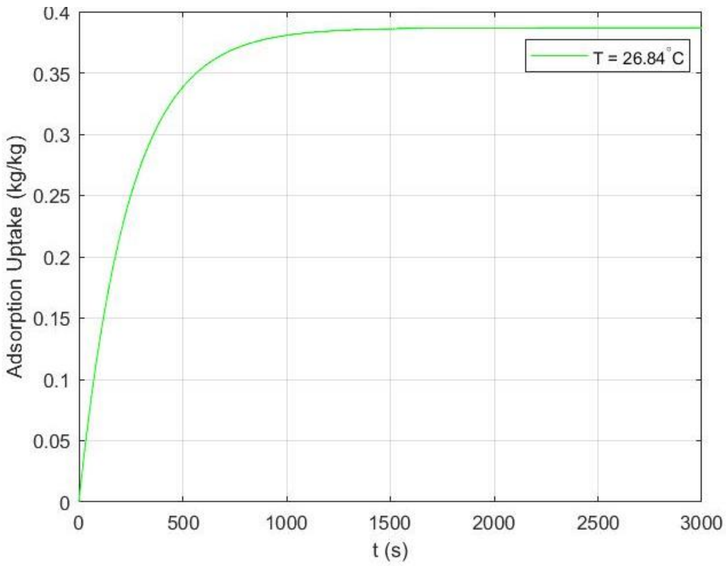

Figure 3. Adsorption kinetic

The kinetic characteristic of the adsorption process highlights the RD–type silica gel adsorbent's ability to absorb water vapor quickly. In this study, the adsorbent was exposed to conditions of 26.84 °C temperature and 60% relative humidity, with an equilibrium absorption value of 0.3876 kg/kg. Under these specific conditions, the RD–type silica gel adsorbent demonstrated a swift absorption rate, initially absorbing 0.38 kg/kg of water vapor within a mere 980 seconds. However, as the absorption process continued, there was a noticeable decrease in the rate of increase in absorption, indicating a gradual saturation of the adsorbent. This finding underscores the adsorbent's effectiveness in rapidly regulating humidity levels, particularly in environments with conditions similar to those in the study. It provides valuable insights into its practical applications for moisture management.

3.3 Heat transfer

In the modeling layer used in this research, there are four layers consisting of air, cloth, silica gel, and the air gap between the silica gel and the surface of the clothes. Each of these layers has heat and mass transfer phenomena, which are calculated according to the conditions and limits determined using Equations 1-4. Variations used in layer modeling are thickness variations, namely at 0.3 mm and 1 mm. Figure 4 depicts the heat transfer rate (Q) for thickness variations of 0.3 mm and 1 mm in the four layers. The heat transfer rate curve is known from the convection and conduction heat transfer rates obtained from previous calculations wherein the phenomenon of convection heat transfer occurs in the first and fourth layers. In the second and third layers, a conduction heat transfer phenomenon occurs.

Figure 4 shows the heat transfer rate value obtained in the four layers. In Figure 4, for a thickness variation of 0.3 mm, it can be seen that there is a decrease in the value from the first layer to the fourth layer, with each value sequentially in the first to fourth layers being 448, 435.2, 434.13 and 425, 32. For a thickness variation of 1 mm, it can be seen that there is a decrease in the value from the first layer with a value of 448 and the second layer with a value of 441.8. The third layer has a value of 441.6, and the fourth is 435.51, while the second and third values of the heat transfer rate do not change. It is because, in solids, less heat is transferred. The decrease in the temperature value from the first to the fourth layer causes the value curve to decrease along with the temperature value in the layer. The reduction in the value is also due to convection heat being channeled more efficiently than by conduction. Based on the comparison of variations of 0.3 mm and 1 mm, the greater the thickness of the layer, the higher the value.

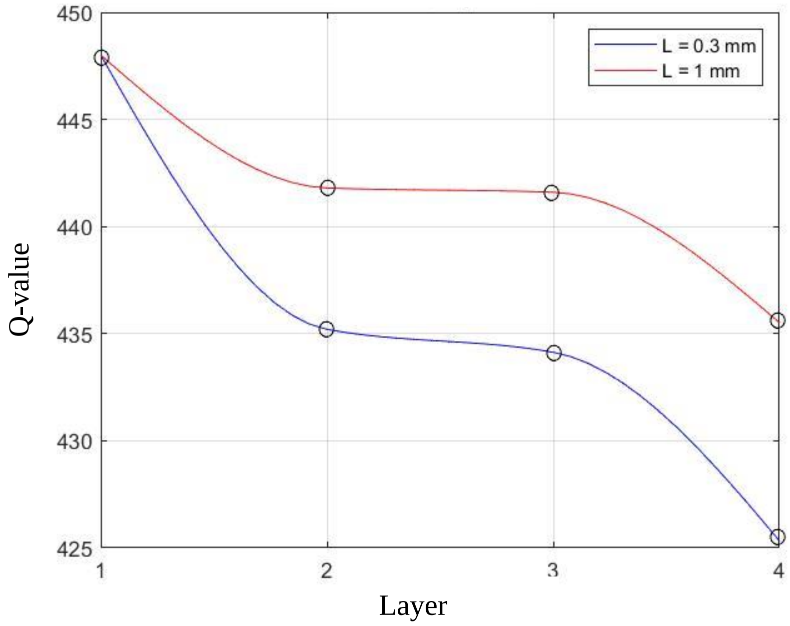

Figure 4. Heat transfer rate comparison

4 Conclusions

The research findings revealed key characteristics of RD–type silica gel as an adsorbent in both isothermal and kinetic adsorption processes conducted at a temperature of 26.84 ℃. In terms of its isothermal behavior, silica gel exhibits an impressive adsorption capacity that ranges from 0.0828 kg/kg at a relative pressure of 0.1 to a remarkable 0.6158 kg/kg at a relative pressure of 0.9. Its performance at a relative humidity of 60% or a relative pressure of 0.6 is particularly noteworthy, with silica gel type RD demonstrating a significant adsorption capacity of 0.3867 kg/kg. The kinetic characteristics of silica gel type RD were derived based on the equilibrium absorption value observed at 60% relative humidity, which stands at 0.3867 kg/kg. Under these specific conditions, the RD–type silica gel adsorbent displays rapid water vapor absorption, initially taking up 0.38 kg/kg within a short span of 980 seconds. However, as the adsorption process continued, there was a noticeable decline in the rate of absorption increase, indicating a gradual saturation of the adsorbent. These findings underscore the remarkable adsorption capabilities of RD–type silica gel, particularly in regulating humidity levels in environments resembling those examined in the study. This research is a pivotal step in advancing the performance of PPE by shedding light on the adsorption properties of RD–type silica gel. It not only benefits the design and functionality of protective equipment, but it also plays a vital role in ensuring the safety, comfort, and well-being of those who rely on it.

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