

Research Article

CO₂ and SO₂ Pressure-Driven Adsorption by 3D Graphene Nanoslits: A Molecular Dynamics Study

Amanda Caroline Borges,¹ Mateus H. Köhler ,² and José Rafael Bordin ^{1,3}

¹Campus Caçapava do Sul, Universidade Federal do Pampa, 96570-000 Caçapava do Sul, Brazil

²Departamento de Física, Universidade Federal de Santa Maria, 97105-900 Santa Maria, Brazil

³Departamento de Física, Instituto de Física e Matemática, Universidade Federal de Pelotas, PO Box 354, 96001-970 Pelotas, Brazil

Correspondence should be addressed to José Rafael Bordin; jrbordin@ufpel.edu.br

Received 21 September 2018; Revised 26 November 2018; Accepted 14 February 2019; Published 18 April 2019

Academic Editor: Renyun Zhang

Copyright © 2019 Amanda Caroline Borges et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

Nonequilibrium molecular dynamics simulations are employed to study the adsorption and blockage properties of a 3D graphene membrane. Specifically, we are interested in the mixtures of carbon dioxide (CO₂) and sulfur dioxide (SO₂), two of the most relevant pollutant gases for the anthropogenic effect in global warming. We simulate cases with distinct proportion of gases in the mixture. Our results indicate that the 3D graphene slit is able to absorb 90% or more of the gas molecules. We show that this property came from the fact that both CO₂ and SO₂ molecules are attracted by the graphene pore, which compensates for the entropic barrier that exists when leaving the bulk state to the confined state. Also, the simulation results show that changing the interlayer separation between the graphene sheets is possible in order to change the membrane properties, from absorbent to blockage. These results help to understand the properties of 3D graphene nanoslits and their application as highly selective filters.

1. Introduction

The demand for clean energy and global warming stand among the major challenges of our time and require extensive investigation towards technological advances. However, while renewable energy often demands massive investments, coal is the least expensive and widespread fossil fuel across the globe, specially in developing countries [1]. On the other hand, burning coal in electric power plants is a major source of carbon dioxide (CO₂) emissions [2]. Even after the combustion gases have passed through macroscopically refined membranes before exiting the smokestack, they contain oxides of nitrogen and sulfur dioxide that lead to smog and acid rain [3]. Reducing the coal-derived emissions, such as CO₂ and SO₂, is, therefore, timely and environmentally imperative.

Nanotechnology represents a huge step in this direction, providing the possibility of high gas selectivity and storage. The capture of gases such as CO₂ and SO₂ is critical for the control and reduction of emissions of pollutant gases.

Graphene and graphene-based materials have attracted great attention in the last decades due to their potential applications in molecular sieves, gas sensing, and energy storage. The large specific surface area (~3000 m²/g⁴) and versatile modification make them excellent adsorbents. A three-dimensional porous graphene can exhibit even higher specific surface area. Ganesan and Shaijumon [4], for instance, synthesized nanoporous graphene with a specific surface area of 3240 m²/g and total pore volume of 2.23 cm³/g. A similar specific surface area has been obtained for 3D graphene samples [5].

Experiments have indicated rather low hydrocarbon uptake by 2D graphene [6]. 3D graphene created through activation processes can enhance its adsorption properties. For instance, an activated graphene-derived carbon exhibited an adsorption of 11.3 mmol/g of CH₄ at room temperature and 35 bar [4]. The introduction of suitable micro- and nanopores can also be important for the adsorption of CO₂ and methane. Chandra et al. have found an impressive adsorption of 4.3 mmol/g of CO₂ in highly microporous

activated graphene [7]. In fact, the combination of multi-layered 3D graphene membranes with nanopores has been used in desalination [8] and molecular separation [9] and in biomolecular and gas sensors [10, 11].

Recent computational studies have contributed to shed some light on the adsorption properties of mixtures of pollutant gases in carbon-based membranes, as disordered carbon [12] and porous aromatic frameworks [13]. Carbon nanotubes were proposed as filters for mixtures of CO_2 and SO_2 [14], showing good adsorption rates [15–17]. In these cases, the main part of the adsorption occurs in the outside of the nanotubes—the optimal pore size for capture is small [18]—and controlling the nanotube radius is an experimental challenge that has not been achieved yet.

Since the adsorption of CO_2 and SO_2 occurs on the surface of the carbon materials, an alternative is the use of graphene, the carbon-based material with the highest available surface area that shows good adsorption properties [19–22]. Among the graphene-based structures, 3D membranes made of stacked porous membrane have been proposed for several applications, which includes water desalination [23–25], water-ethanol separation [26], chemical protection [27], and gas separation [28].

In the specific case of CO_2 , experimental studies have shown that these molecules are adsorbed in the graphene sheet [29–31]. However, as far as we know, there are no experimental studies on the adsorption of a mixture of CO_2 and SO_2 in graphene. In order to better understand this subject, in this paper, we study the adsorbing properties of a 3D porous graphene membrane when a CO_2 and SO_2 mixture is pushed through the membrane by an external pressure-driven force. Our goal is to obtain information on how 3D graphene structures can be employed as selective and, principally, effective filters for CO_2 and SO_2 gases. Our results indicate a high adsorption, with the membrane acting as a sponge that absorbs 90% or more of the gas molecules. Also, by changing the interlayer distance between the graphene sheets, we can change the membrane from an adsorbent to a blocker, with no gas passing through it. This change in the distance can be experimentally done varying the type and amount of reducer used in the graphene chemical production [32, 33]. This feature makes it more experimentally attainable than controlling the radius of produced nanotubes.

Our paper is organized as follows. In Section 2, we present the computational details of our simulations. The results and discussions are shown in Section 3, while the conclusions are done in Section 4.

2. Computational Details

Our gaseous system consists in 1000 CO_2 and SO_2 molecules initially placed at the left of the simulation box, as shown in Figure 1. A pressure gradient (ΔP) forces the solution against the nanoporous membrane located at the center of the box with dimensions $5 \times 5 \times 20$ nm in the x , y , and z directions. The membrane consists of three graphene sheets, each one with randomly distributed nanogaps. The interlayer separation (d_z) was set to 1 nm and the nanogap size range from

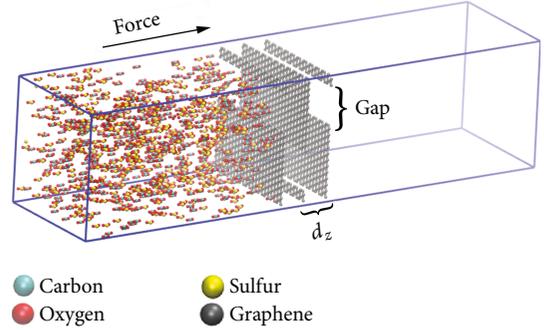


FIGURE 1: Schematic representation of the simulation framework. The system is divided as follows: on the left side, we can see the CO_2 and SO_2 molecules initially placed in a random position, while at the center of the box, we have the graphene nanoslits.

TABLE 1: The Lennard-Jones parameters and charges of the simulated atoms. The crossed parameters were obtained by the Lorentz-Berthelot rule.

Atomic species	σ (nm)	ϵ (kB)	Charge
C (CO_2) [20]	0.280	27.0	0.70
O (CO_2) [20]	0.301	79.0	-0.35
S (SO_2) [38]	0.358	154.0	0.47
O (SO_2) [38]	0.299	62.3	-0.235
C (graphene)	0.340	78.0	0.0

0.5 to 2 nm. Due to the simulation time scale (10 ns), we used 100 MPa as the standard ΔP , higher than the osmotic pressure used in the experiments (0.1 to 30 MPa [34]), because low pressures yield low gas fluxes that would not go above the statistical error.

To study the influence of distinct gas mixtures, we employed simulations with distinct gas fractions $\varphi = 1 - n_{\text{CO}_2}/n_{\text{SO}_2}$, where n_{CO_2} and n_{SO_2} stand for the number of CO_2 and SO_2 molecules, respectively.

The SHAKE algorithm [35] was employed to maintain the rigidity of CO_2 and SO_2 molecules. Nonbonded interactions are described by the Lennard-Jones (LJ) potential with a cut-off distance of 1 nm, and the parameters are tabulated in Table 1. The Lorentz-Berthelot mixing rule [36] was used to obtain the LJ parameters for different atomic species. The long-range electrostatic interactions were calculated by the *Particle-Particle Particle-Mesh* method [37], and periodic boundary conditions were applied in all directions.

For each nonequilibrium simulation with nanopores, the system was first equilibrated in the NVT ensemble for 1 ns at $T = 300$ K. During equilibration, the graphene atoms were held fixed in space and a repulsive plug prevented the gas molecules from entering the nanoslit. After equilibration, the plug is removed and the pressure gradient is applied to characterize the gas flux through the nanopores. We carried out five independent simulations for each system collecting the trajectories of atoms every picosecond for 10 ns. All

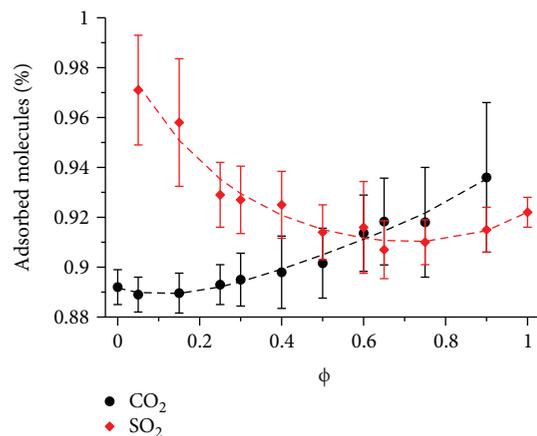


FIGURE 2: Variation of the percentage of molecules adsorbed by the graphene nanoslits for distinct fraction mixtures of CO_2/SO_2 .

molecular dynamics simulations were implemented within the Extensible Software Package for Research on Soft Matter (ESPresSO) [39, 40].

3. Results and Discussion

3.1. Gas Adsorption: The Influence of Molar Fraction. Environmentally friendly companies aim to reduce their CO_2 emissions through dedicated membranes that selectively filter the impurities from the air. In the coal-based industry, it is particularly complicated to separate the carbon from the sulfur dioxide coming from the burning fossil fuel. Therefore, the membrane's ability of effectively recovering the mixture of CO_2 and SO_2 is crucial. It is usually associated with the percentage of gas molecules adsorbed by the membrane.

In Figure 2, we show the percentage of molecules trapped inside the graphene nanoslits or adsorbed at the graphene walls as a function of the CO_2 and SO_2 fraction. When $\phi = 0$, there are only CO_2 molecules in the system, while for $\phi = 1$, only SO_2 are present. By varying this fraction, we notice a blockage higher than 88% for all the samples. Markedly, for $\phi = 0.5$ (50% of each species), we observed higher SO_2 blockage compared with the CO_2 , which highlights the sulfur dioxide selectivity of the membrane. This is an important result as SO_2 is the main ingredient of acid rain. Also, both gases have high adsorption, which is a direct result of the graphene's high available surface area. It prevents one of the main problems in current filters, where SO_2 is blocked and the CO_2 escapes to the atmosphere [12].

In order to analyze the adsorption dynamics, we plot in Figure 3 the percentage of adsorbed molecules as a function of time. Figure 3(a) shows the situation in which we have only CO_2 or SO_2 , while Figure 3(b) refers to the 50% mixture. Both situations show similar adsorption dynamics, with sulfur dioxide being fully adsorbed for longer times: it reaches a plateau of $\sim 90\%$ in adsorption after 2 ns, while CO_2 takes only 1 ns. Sulfur atoms are larger and their electronegativity makes SO_2 much more polar than CO_2 , which is a determinant for the entropic barrier at the nanopore

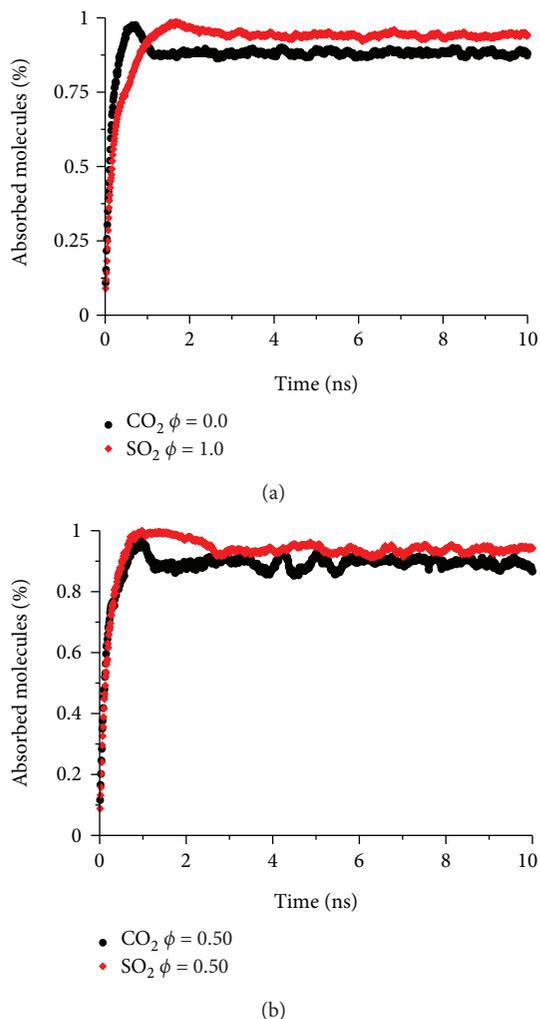


FIGURE 3: Percentage of molecules adsorbed by the graphene nanoslits as a function of the simulation time for distinct fractions.

entrance as it goes from the bulk to the nanoconfined state. This entropic penalty occurs since the entropy is higher in the bulk state, while inside the Nanoslit, there is a decrease in the entropy due to the geometric constriction [41]. It would explain the slightly larger adsorption rate of SO_2 in Figure 3(a). Markedly, both carbon and sulfur dioxides are highly adsorbed by the graphene nanoslits and remain inside the slits, even under a large pressure gradient $\Delta P = 100$ MPa. The oscillations observed after 2 ns originated from the method used to calculate the number of adsorbed molecules. If the central atom of one molecule outside the nanopore—C for CO_2 or S for SO_2 —was closer than the interatomic separation, given by the σ in Table 1, it was considered as adsorbed. Due to the thermal fluctuations, the adsorbed atom position can fluctuate beyond the *cut-off* employed in our methodology, leading to fluctuations around the mean value of the percentage of adsorbed molecules. Increasing the *cut-off* could lead to less fluctuations but also to spurious results, since it could account for atoms that are not adsorbed in the external surface of the graphene nanopore.

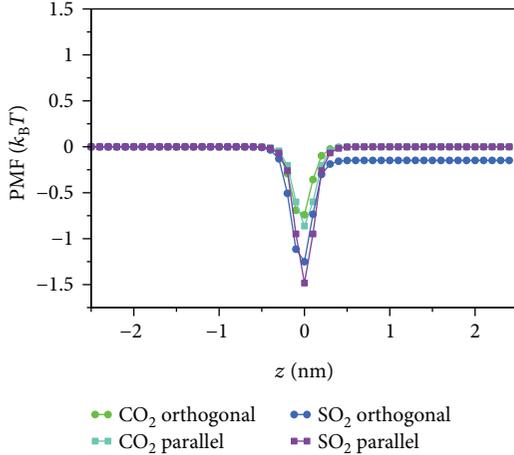


FIGURE 4: Potential of mean force (PMF) of CO_2 and SO_2 molecules as a function of the distance from the graphene nanoslit. Two molecular conformations are considered: parallel and orthogonal to the graphene surface. The energy is measured as a function of the thermal energy $k_B T$, where $k_B = 1.38 \text{ J/K}$ is the Boltzmann constant and $T = 300 \text{ K}$ is the system temperature.

The conjunction of forces acting on the nanoscale leads to most varied behaviors in fluid dynamics. The entropic contribution to the water molecules leaving the bulk reservoir and entering the nanopore is also relevant [42]. In order to understand how these phenomena are affecting our system, we plot in Figure 4 the potential of mean force (PMF) of a single molecule as a function of the distance between the molecule and the nanoporous graphene. The changes in the PMF as a function of the intermolecular distances provide qualitative insights on the attractive/repulsive nature of the interaction. For this evaluation, we consider only one graphene sheet placed at the center of the simulation box. The molecule is pulled through the center of the slit, and the force is evaluated at each 0.1 nm and then integrated to obtain the PMF. The results show that regardless of the molecular orientation (if parallel or orthogonal to the graphene surface), both molecules (CO_2 and SO_2) are attracted to the nanopore. Interestingly, the carbon dioxide presents half of the attraction (~ 0.8) suffered by the sulfur compound (~ 1.5) in the vicinity of the graphene nanopore. In other words, the dense packing at the graphene interface observed in Figure 5(b) and the high adsorption rate of SO_2 in Figure 3 can be explained in terms of the attraction between the SO_2 molecules and the graphene nanopore. The combination of these factors with the pressure gradient applied to the solution makes the graphene nanoslits very promising for the adsorption of CO_2 and SO_2 .

In the nanoscaled flow, the molecular structure is often a determinant for the fluid dynamics: as the molecules get together to form highly packed structures (e.g., at graphene interfaces [43], in nanotubes [44], and in zeolites [45]), the molecular structure slows down the flux. In order to investigate the impact of the molecular structure in the adsorption of CO_2 and SO_2 , we plot in Figure 5 the density profile of both species along the simulation

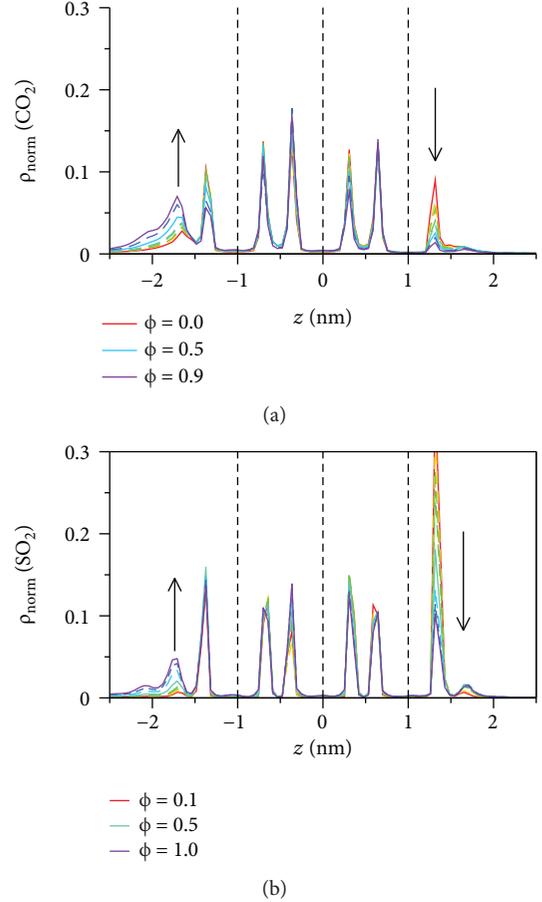


FIGURE 5: Density profiles of (a) CO_2 and (b) SO_2 for different ϕ inside and near the graphene nanoslit. The dotted lines represent the graphene layer positions.

box (z direction). Once the densities are different, we plot the normalized density

$$\rho_{\text{norm}}(z) = \frac{\rho(z)}{\int \rho(z) dz}. \quad (1)$$

From Figure 5(a), we can observe sharp, dense peaks between the graphene nanoslits, indicating a high adsorption rate of CO_2 . As we increase the fraction ϕ of SO_2 in the solution, we observe an increase in the number of CO_2 molecules rejected by the graphene nanopore, as can be seen by the increase in the first peak (left) and the density deflation at the right of the graphene layers.

In Figure 5(b), we found the SO_2 molecules arranged in a very densely packed structure close to the third graphene sheet (in the opposite direction of the applied pressure) for small fractions ϕ of SO_2 . Conversely, as we increase ϕ , the sulfur dioxide molecules become more homogeneously distributed at the graphene interfaces. This aggregation at the graphene surface is important either for the separation of CO_2 and SO_2 or for the storage of these substances.

3.2. Gas Adsorption: The Influence of Interlayer Separation. The geometry of the nanopore is determinant for the

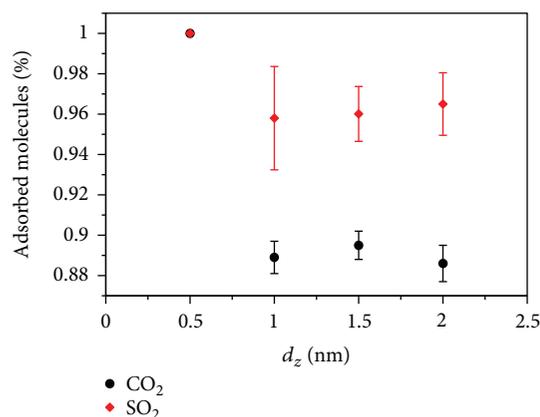


FIGURE 6: Adsorption for the distinct interlayer separation d_z in a system with fraction $\phi = 0.25$.

structural and dynamical properties of the confined fluid. In nanotubes, for instance, a change in the diameter can produce phase transitions at ambient pressure and temperature [46, 47]. The same is valid for 2D confinement of fluids. A small variation in the interlayer distance of graphene can promote dynamical anomalies in the fluid viscosity [48] and diffusion [49] and even in their phase diagram [50]. Additionally, the interlayer separation (d_z) yields important consequences on the graphene membrane's adsorption capacity [51, 52].

In Figure 6, we show the adsorption as a function of the interlayer separation d_z for a system with fraction $\phi = 0.25$. If the interlayer separation is smaller than 1.0 nm, such as 0.5 nm, the particles are not absorbed by the nanoslit but blocked by it, as we can see in Figures 7(a) and 7(b). The inner space is so small that the molecules get blocked between the second and third graphene layers. Interestingly, if only one graphene sheet is used (a 2D membrane), the gas would pass, once it crosses through the first graphene layer in our system. Nevertheless, this result indicates that a 3D graphene membrane can block the passage of gases. On the other hand, for interlayer separations between 1.0 nm and 2.0 nm, the adsorption and the structure are not affected by d_z , as we can see in the results shown in Figures 6 and 7. Therefore, we can easily change the properties of the 3D graphene filter just by varying d_z : if $d_z > 1.0$ nm, it works as a sponge that absorbs both CO₂ and SO₂, while if $d_z < 1.0$ nm, it blocks the gas passage. This blockage happens due to geometric effects—the interlayer distance 0.5 nm is comparable to the excluded volume of the molecules.

4. Summary and Conclusions

In this work, we investigated the CO₂ and SO₂ absorption properties of graphene nanoslits using molecular simulations. Our results indicate that 3D graphene membranes are a promising material for selective filters, absorbing both gases with more than 90% efficiency. Also, it is more selective for sulfur dioxide, as we show by the PMF calculations. Also, we show that by controlling the interlayer separations, the

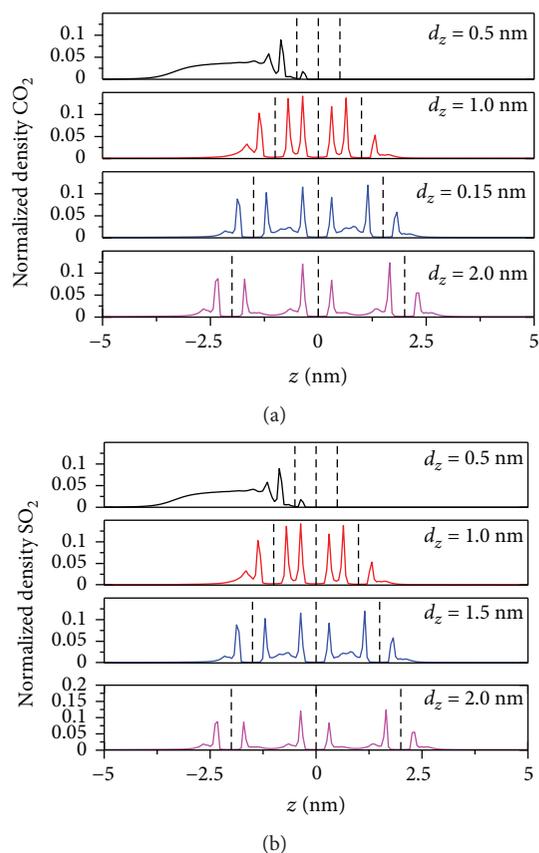


FIGURE 7: Density profiles of (a) CO₂ and (b) SO₂ inside and near the nanoslit for different interlayer separations d_z . The dotted lines represent the graphene layer positions in each case.

3D membrane can be used either as an absorbing filter or as a blocking filter, where no gas can pass through the membrane. The 3D characteristic of the graphene nanoslits is essential to ensure the blockage, as our analysis has shown. These results indicate that 3D graphene structures are promising filters for pollutant gases, with high selectivity and efficiency.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflict of interest.

Acknowledgments

The authors acknowledge the Brazilian agencies CAPES, CNPq, and FAPERGS for the financial support.

References

- [1] D. Tong, Q. Zhang, S. J. Davis et al., "Targeted emission reductions from global super-polluting power plant units," *Nature Sustainability*, vol. 1, no. 1, pp. 59–68, 2018.

- [2] H.-L. Chang, C. M. Chen, C. H. Sun, and H. D. Lin, "Carbon footprint of automotive ignition coil," *IOP Conference Series: Materials Science and Engineering*, vol. 87, article 012016, 2015.
- [3] P. Amiotte Suchet, A. Probst, and J. L. Probst, "Influence of acid rain on CO₂ consumption by rock weathering: local and global scales," *Water, Air, and Soil Pollution*, vol. 85, no. 3, pp. 1563–1568, 1995.
- [4] A. Ganesan and M. M. Shaijumon, "Activated graphene-derived porous carbon with exceptional gas adsorption properties," *Microporous and Mesoporous Materials*, vol. 220, pp. 21–27, 2016.
- [5] L. Zhang, F. Zhang, X. Yang et al., "Porous 3D graphene-based bulk materials with exceptional high surface area and excellent conductivity for supercapacitors," *Scientific Reports*, vol. 3, no. 1, article 1408, 2013.
- [6] B. Szcześniak, J. Choma, and M. Jaroniec, "Gas adsorption properties of graphene-based materials," *Advances in Colloid and Interface Science*, vol. 243, pp. 46–59, 2017.
- [7] V. Chandra, S. U. Yu, S. H. Kim et al., "Highly selective CO₂ capture on N-doped carbon produced by chemical activation of polypyrrole functionalized graphene sheets," *Chemical Communications*, vol. 48, no. 5, pp. 735–737, 2012.
- [8] D. Cohen-Tanugi, L.-C. Lin, and J. C. Grossman, "Multilayer nanoporous graphene membranes for water desalination," *Nano Letters*, vol. 16, no. 2, pp. 1027–1033, 2016.
- [9] P. Wang, W. Li, C. du et al., "CO₂/N₂ separation via multilayer nanoslit graphene oxide membranes: molecular dynamics simulation study," *Computational Materials Science*, vol. 140, pp. 284–289, 2017.
- [10] S. Garaj, S. Liu, J. A. Golovchenko, and D. Branton, "Molecule-hugging graphene nanopores," *Proceedings of the National Academy of Sciences of the United States of America*, vol. 110, no. 30, pp. 12192–12196, 2013.
- [11] W. Wei, J. Nong, L. Tang, G. Zhang, J. Yang, and W. Luo, "Conformal graphene-decorated nanofluidic sensors based on surface plasmons at infrared frequencies," *Sensors*, vol. 16, no. 6, p. 899, 2016.
- [12] X. Peng, S. K. Jain, and J. K. Singh, "Adsorption and separation of N₂/CH₄/CO₂/SO₂ gases in disordered carbons obtained using hybrid reverse Monte Carlo simulations," *Journal of Physical Chemistry C*, vol. 121, no. 25, pp. 13457–13473, 2017.
- [13] D. Zhang, X. Jing, D. S. Sholl, and S. B. Sinnott, "Molecular simulation of capture of sulfur-containing gases by porous aromatic frameworks," *Journal of Physical Chemistry C*, vol. 122, no. 32, pp. 18456–18467, 2018.
- [14] S. K. Dash, "Post combustion carbon dioxide capture using amine functionalized carbon nanotubes: a review," *AIP Conference Proceedings*, vol. 1724, no. 1, article 020117, 2016.
- [15] M. Rahimi, J. K. Singh, and F. Müller-Plathe, "Adsorption and separation of binary and ternary mixtures of SO₂, CO₂ and N₂ by ordered carbon nanotube arrays: grand-canonical Monte Carlo simulations," *Physical Chemistry Chemical Physics*, vol. 18, no. 5, pp. 4112–4120, 2016.
- [16] D. J. Babu and J. J. Schneider, "Gas adsorption studies of CO₂ in carbon nanomaterials: a case study of vertically aligned carbon nanotubes," *Chemie Ingenieur Technik*, vol. 89, no. 10, pp. 1273–1287, 2017.
- [17] Y.-B. Yang, M. Rahimi, J. K. Singh, M. C. Böhm, and F. Müller-Plathe, "Adsorption and condensation of SO₂ in double-walled carbon nanotube arrays studied by Monte Carlo simulations and simple analytical models," *The Journal of Physical Chemistry C*, vol. 120, no. 14, pp. 7510–7521, 2016.
- [18] S. Wang, Z. Tian, S. Dai, and D.-e. Jiang, "Optimal size of a cylindrical pore for post-combustion CO₂ capture," *The Journal of Physical Chemistry C*, vol. 121, no. 40, pp. 22025–22030, 2017.
- [19] Y. Jiang, S. Yang, S. Li, W. Liu, and Y. Zhao, "Highly sensitive CO gas sensor from defective graphene: role of van der Waals interactions," *Journal of Nanomaterials*, vol. 2015, Article ID 504103, 7 pages, 2015.
- [20] Y. Liu and J. Wilcox, "Molecular simulation studies of CO₂ adsorption by carbon model compounds for carbon capture and sequestration applications," *Environmental Science & Technology*, vol. 47, no. 1, pp. 95–101, 2012.
- [21] M. Maurya and J. K. Singh, "A grand canonical Monte Carlo study of SO₂ capture using functionalized bilayer graphene nanoribbons," *The Journal of Chemical Physics*, vol. 146, no. 4, article 044704, 2017.
- [22] M. Maurya and J. K. Singh, "Treatment of flue gas using graphene sponge: a simulation study," *The Journal of Physical Chemistry C*, vol. 122, no. 26, pp. 14654–14664, 2018.
- [23] M. Dahanayaka, B. Liu, Z. Hu et al., "Graphene membranes with nanoslits for seawater desalination via forward osmosis," *Physical Chemistry Chemical Physics*, vol. 19, no. 45, pp. 30551–30561, 2017.
- [24] B. Chen, H. Jiang, X. Liu, and X. Hu, "Molecular insight into water desalination across multilayer graphene oxide membranes," *ACS Applied Materials & Interfaces*, vol. 9, no. 27, pp. 22826–22836, 2017.
- [25] M. H. Köhler, J. R. Bordin, and M. C. Barbosa, "Ion flocculation in water: from bulk to nanoporous membrane desalination," *Journal of Molecular Liquids*, vol. 277, pp. 516–521, 2019.
- [26] S. Gravelle, H. Yoshida, L. Joly, C. Ybert, and L. Bocquet, "Carbon membranes for efficient water-ethanol separation," *The Journal of Chemical Physics*, vol. 145, no. 12, article 124708, 2016.
- [27] R. Spitz Steinberg, M. Cruz, N. G. A. Mahfouz, Y. Qiu, and R. H. Hurt, "Breathable vapor toxicant barriers based on multilayer graphene oxide," *ACS Nano*, vol. 11, no. 6, pp. 5670–5679, 2017.
- [28] H. Cheng and G. Lei, "Multilayer graphene nanostructure separate CO₂/CH₄ mixture: combining molecular simulations with ideal adsorbed solution theory," *Chemical Physics Letters*, vol. 661, pp. 31–35, 2016.
- [29] A. Ghosh, K. S. Subrahmanyam, K. S. Krishna et al., "Uptake of H₂ and CO₂ by graphene," *The Journal of Physical Chemistry C*, vol. 112, no. 40, pp. 15704–15707, 2008.
- [30] K. Takeuchi, S. Yamamoto, Y. Hamamoto et al., "Adsorption of CO₂ on graphene: a combined TPD, XPS, and vdW-DF study," *Journal of Physical Chemistry C*, vol. 121, no. 5, pp. 2807–2814, 2017.
- [31] E. Singh, M. Meyyappan, and H. S. Nalwa, "Flexible graphene-based wearable gas and chemical sensors," *ACS Applied Materials & Interfaces*, vol. 9, no. 40, pp. 34544–34586, 2017.
- [32] W. Chen and L. Yan, "In situ self-assembly of mild chemical reduction graphene for three-dimensional architectures," *Nanoscale*, vol. 3, no. 8, pp. 3132–3137, 2011.
- [33] S. V. Tkachev, E. Y. Buslaeva, A. V. Naumkin, S. L. Kotova, I. V. Laure, and S. P. Gubin, "Reduced graphene oxide," *Inorganic Materials*, vol. 48, no. 8, pp. 796–802, 2012.

- [34] D. Chen, J.-Q. Shi, S. Durucan, A. Korre, and A. Syed, "12th International Conference on Greenhouse Gas Control Technologies, GHGT-12," *Energy Procedia*, vol. 63, article 4630, 2014.
- [35] J.-P. Ryckaert, G. Ciccotti, and H. J. C. Berendsen, "Numerical integration of the Cartesian equations of motion of a system with constraints: molecular dynamics of n-alkanes," *Journal of Computational Physics*, vol. 23, no. 3, pp. 327–341, 1977.
- [36] M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, Oxford University Press, Oxford, 1987.
- [37] R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles*, McGraw-Hill, New York, 1981.
- [38] M. C. C. Ribeiro, "Molecular dynamics simulation of liquid sulfur dioxide," *The Journal of Physical Chemistry. B*, vol. 110, no. 17, pp. 8789–8797, 2006.
- [39] H.-J. Limbach, A. Arnold, B. A. Mann, and C. Holm, "ESPReso—an extensible simulation package for research on soft matter systems," *Computer Physics Communications*, vol. 174, no. 9, pp. 704–727, 2006.
- [40] A. Arnold, O. Lenz, S. Kesselheim et al., "ESPReso 3.1: molecular dynamics software for coarse-grained models," in *Meshfree Methods for Partial Differential Equations VI*, M. Griebel and M. A. Schweitzer, Eds., vol. 89 of Lecture Notes in Computational Science and Engineering, pp. 1–23, Springer, Berlin, Heidelberg, 2013.
- [41] J. R. Bordin, A. Diehl, M. C. Barbosa, and Y. Levin, "Ion fluxes through nanopores and transmembrane channels," *Physical Review E*, vol. 85, no. 3, article 031914, 2012.
- [42] M. H. Köhler, J. R. Bordin, and M. C. Barbosa, "2D nanoporous membrane for cation removal from water: effects of ionic valence, membrane hydrophobicity, and pore size," *The Journal of Chemical Physics*, vol. 148, no. 22, article 222804, 2018.
- [43] G. Cicero, J. C. Grossman, E. Schwegler, F. Gygi, and G. Galli, "Water confined in nanotubes and between graphene sheets: a first principle study," *Journal of the American Chemical Society*, vol. 130, no. 6, pp. 1871–1878, 2008.
- [44] M. H. Köhler and J. R. Bordin, "Surface, density, and temperature effects on the water diffusion and structure inside narrow nanotubes," *The Journal of Physical Chemistry C*, vol. 122, no. 12, pp. 6684–6690, 2018.
- [45] S. H. Jamali, T. J. H. Vlugt, and L.-C. Lin, "Atomistic understanding of zeolite nanosheets for water desalination," *Journal of Physical Chemistry C*, vol. 121, no. 21, pp. 11273–11280, 2017.
- [46] K. V. Agrawal, S. Shimizu, L. W. Drahushuk, D. Kilcoyne, and M. S. Strano, "Observation of extreme phase transition temperatures of water confined inside isolated carbon nanotubes," *Nature Nanotechnology*, vol. 12, no. 3, pp. 267–273, 2017.
- [47] M. H. Köhler, J. R. Bordin, L. B. da Silva, and M. C. Barbosa, "Breakdown of the Stokes–Einstein water transport through narrow hydrophobic nanotubes," *Physical Chemistry Chemical Physics*, vol. 19, no. 20, pp. 12921–12927, 2017.
- [48] M. Neek-Amal, F. M. Peeters, I. V. Grigorieva, and A. K. Geim, "Commensurability effects in viscosity of nanoconfined water," *ACS Nano*, vol. 10, no. 3, pp. 3685–3692, 2016.
- [49] L. B. Krott, J. R. Bordin, N. M. Barraz Jr., and M. C. Barbosa, "Effects of confinement on anomalies and phase transitions of core-softened fluids," *The Journal of Chemical Physics*, vol. 142, no. 13, article 134502, 2015.
- [50] J. R. Bordin, L. B. Krott, and M. C. Barbosa, "Surface phase transition in anomalous fluid in nanoconfinement," *Journal of Physical Chemistry C*, vol. 118, no. 18, pp. 9497–9506, 2014.
- [51] R. S. Rajaura, S. Srivastava, V. Sharma et al., "Role of interlayer spacing and functional group on the hydrogen storage properties of graphene oxide and reduced graphene oxide," *International Journal of Hydrogen Energy*, vol. 41, no. 22, pp. 9454–9461, 2016.
- [52] B. H. Kim, W. G. Hong, H. Y. Yu et al., "Thermally modulated multilayered graphene oxide for hydrogen storage," *Physical Chemistry Chemical Physics*, vol. 14, no. 4, pp. 1480–1484, 2012.



Hindawi
Submit your manuscripts at
www.hindawi.com

