Grand Canonical Monte Carlo Modeling of Anesthetic Xe Separation from Exhale Gas Mixtures Using Metal Organic Frameworks

Yeliz GURDAL[*]

Department of Bioengineering, Adana Alparslan Turkes Science and Technology University, Turkey

Abstract

Xe has been shown to be a promising candidate for anesthetic applications. However, its high price prevents its usage in clinical industry. An alternative approach is to recover Xe from anesthetic exhale gas mixture and recycle it to the inhale gas stream. Although, many membranes and/or adsorbents have been proposed for recovering anesthetic Xe, using metal organic frameworks (MOFs) for adsorption based separation of anesthetic Xe exhale gas mixtures has been newly studied. MOFs have tunable pore sizes, large surface areas, and high porosities which make them potential candidates for gas separation applications. Currently, very little is known about anesthetic Xe recovery performances of MOFs. We theoretically investigate adsorption based separation of single component and binary mixtures of CO_2, Xe, and N_2 in three MOFs, namely CECYOY, SUDBOI, and ZUQPOQ. Single component and binary adsorption isotherms and adsorption selectivities are calculated using Grand Canonical Monte Carlo simulations for each MOF in order to characterize their performances as adsorbents. Results suggest that while MOFs prefer adsorption of CO_2 for CO_2/Xe mixture, Xe adsorption is favorable in the case of Xe/N_2 mixture. While SUDBOI shows significantly large CO_2 adsorption selectivity for CO_2/Xe mixture, ZUQPOQ has the largest adsorption selectivity for Xe/N_2 mixture.

Keywords: Grand Canonical Monte Carlo simulations, metal organic frameworks, gas separation

Metal Organik Çerçeveler Kullanarak Ekshale Gaz Karışımlarından Anestezik Xe Ayrılmasının Grand Canonical Monte Carlo Yöntemi ile Modellenmesi

Öz

Xe'nin anestezi uygulamalarında kullanılabileceği literatürdeki çalışmalarda gösterilmiştir. Fakat, yüksek maaliyeti Xe'nin klinik uygulamalarda kullanımını engellemektedir. Buna çözüm üretebilecek bir yaklaşım olarak, Xe'nin solunum yoluyla verilen anestezik gaz karışımından geri kazanılması ve solunan gaz akımına geri beslenmesi önerilmiştir. Anestetik Xe'nin geri kazanılması için birçok membran ve/veya adsorban önerilmiş olsa da, anestezik Xe'nin metal organik kafes yapılar (MOF) kullanılarak geri kazanılması yeni çalışılmaya başlanan bir konudur. MOF'ların gaz ayırma uygulamalarında kullanılmalarına olanak veren özellikleri ayarlanabilir gözenek boyutlarına, geniş yüzey alanlarına ve yüksek gözenekli yapıya sahip olmalarıdır. Literatürde MOF'ların anestezik Xe gazını geri kazanım performansları hakkında sınırlı sayıda çalışma vardır. Çalışmamızda CECYOY, SUDBOI, and ZUQPOQ isimli MOF'ların tek bileşenli ve ikili CO_2, Xe ve N_2 karışımlarını adsorpsiyon bazlı ayırma performansları incelenmiştir. Gazların tekli ve karışım halindeki adsorpsiyon izotermleri ve adsorpsiyon seçicilikleri her bir MOF için Grand Canonical Monte Carlo simülasyonları kullanılarak hesaplanmıştır. Sonuçlar, MOF'larda CO_2/Xe karışımı için CO_2 adsorpsiyonunun tercih edildiğini, Xe adsorpsiyonunun ise Xe/N_2 karışımı durumunda tercih edildiğini göstermiştir. SUDBOI, CO_2/Xe karışımı için yüksek CO_2 adsorpsiyon seçiciliği gösterirken, ZUQPOQ, Xe/N_2 karışımı için en yüksek Xe adsorpsiyon seçiciliğine sahiptir.

Anahtar Kelimeler: Grand Canonical Monte Carlo Simülasyonu, metal oraganik kafes yapılar, gaz ayırma

*Corresponding Author: ygurdal@atu.edu.tr

1. Introduction

Xenon (Xe), being a noble gas, has several usage in engineering applications including lighting, biomedical imaging, nuclear magnetic resonance, neutron counters (Banerjee et al., 2018). Additionally, Xe is shown to be a potential candidate for anesthetics applications. Xe has high chemical stability, low flammability, low solubility in blood, minimal respiratory side effects, low interactions with drug molecules, which makes it a perfect candidate to be used as an anesthetics (Neice and Zornow, 2016). It can bind to proteins such as myoglobins as well as bilayer lipids through temporary polarization of its electrons (Franks, 2008). Although, Xe is shown to be a promising candidate in anesthetics applications, currently its price is preventing itself from being used as an anesthetic gas. The price of high purity Xe is reported as \$5000 per kilogram (Elsaidi et al., 2017). This significantly high price arises from the cost of obtaining pure Xe, through energetically intensive cryogenic distillation of air. For clinical purposes, though, Xe gas can be recovered from the anesthetic gas mixture and recycled back for further usage.

Some portable Xe recovery devices for clinical usage have been already proposed in the literature. One example is, liquefying Xe at high pressure, 66 bar, and separating it from the exhale gas mixture using soda lime (Georgieff and Bader, 1996). Another study proposes the use of activated carbon at 77 K and slowly boiling of Xe first by increasing the temperature the system (Burov et al., 2000). These methods require high energy and yield high capital and operation costs, thus preventing re-use of the Xe gas in the medical industry. Proposing cheap and highly efficient Xe recovery systems becomes important in the development of renewable applications.

Searching for alternative technologies for Xe recovery from anesthetic exhale gas is its infancy period in the literature, thus, deserves further detailed theoretical and/or experimental investigation.

Metal organic frameworks (MOFs) have been shown to be promising nanoporous material candidates for separating Xe from its binary mixtures of Xe/Kr and Xe/Ar (Gurdal and Keskin, 2016; Gurdal and Keskin 2013). The exceptional performances of MOFs for gas separation applications are attributed to their high surface area, high porosity, high chemical/physical stability, and wide range of pore size enabling selective separation of the gas mixtures (Gurdal and Keskin, 2012).

There are a few literature on the Xe recovery from anesthetic gas mixture using MOFs. Elsaidi et al. (2017) have conducted combined experimental and theoretical work to investigate Xe recovery from anesthetic exhale gas mixtures of 65% Xe, 24% O_2, 6% N_2, and 5% CO_2 using MOFs (NiDOBDC, HKUST-1, and PCN-12). According to the results, NiDOBDC, HKUST-1, and PCN-12 have high Xe uptakes of 2.62, 3.62, and 4.4 mmol/g, respectively. Among the others, PCN-12 also shows higher Xe/O_2, Xe/N_2, and Xe/CO_2 adsorption selectivity, which are calculated as 18.25, 18.46, and 1.99, respectively. Wang et al. (2019) have studied DD3R zeolite membranes for selective separation of CO_2 from Xe by experimental and theoretical efforts. Results suggest that DD3R zeolite can be a benchmark membrane providing high diffusion selectivity of CO_2 over Xe. Wang and Kapteijn et al. (2019) have investigated potential usage of MFI zeolite for CO_2/Xe membrane-based separation. They show that MFI zeolite membrane favors CO_2 permeation much higher than Xe which is attributed to facilitated diffusion of CO_2 in

short and straight channels of the b-oriented MFI.

To the best our our knowledge, there has been only three literature addressing recovery of the Xe from anesthetic exhale gas mixture using nanoporous materials. To fill this gap in the literature, our aim is to theoretically investigate adsorption based separation performances of single component and binary mixtures of CO_2, Xe, and N_2 by taking advantage of MOFs, namely CECYOY, SUDBOI, and ZUQPOQ. Grand canonical Monte Carlo (GCMC) simulations are performed in order to determine adsorption of the gas mixtures in corresponding MOFs. In addition to calculating adsorption isotherms, we also calculate adsorption selectivities for determining potential MOFs that can recover Xe from the anesthetic gas mixture selectively and efficiently.

2. Material and Methods

We perform Grand Canonical Monte Carlo (GCMC) (Allen and Tildesley, 1987) simulations to compute adsorption isotherms of single and binary components of anesthetic exhale gas mixtures, such as CO_2, Xe, and N_2 in MOFs having different pore sizes and porosities. We investigate the adsorption behavior of three MOFs, namely CECYOY, SUDBOI, and ZUQPOQ. Structural parameters of the MOFs under consideration are summarized in Table 1.

Table 1. Structural properties of the MOFs considered in this work. PLD and LCD stands for pore limiting diameter and largest cavity diameter, respectively. For more details, see Ref. [13].

MOFs	PLD (Å)	LCD (Å)	Porosity (%)	Density (g/cm³)	Accessible Surface Area (m²/g)
CECYOY	3.34	3.85	38	1.67	26.48
SUDBOI	3.6	6.29	56	1.23	599.8
ZUQPOQ	3.41	4.02	33	1.53	122.49

As it can be seen from the Table 1, SUDBOI has the largest pores with respect to CECYOY and ZUQPOQ. Accordingly, its accessible surface area is the largest one, 599.8 m²/g. CECYOY, on the other hand, possesses the smallest PLD and LCD (Altintas and Keskin, 2017). While, SUDBOI has the largest porosity, 56%, CECYOY and ZUQPOQ show similar porosities, being 38% and 33%, respectively.

Atomic positions of the MOF crystals are taken from the Cambridge Crystallographic Data Centre (CCDC) (Allen, 2002). We assume rigid structures for the MOFs which have been tested and shown as an appropriate simulation strategy for most of the MOFs.

Lennard-Jones (LJ) potentials are used to calculate the gas-gas and gas-MOF atoms interactions (Frenkel and Smit, 1987). Lorentz−Berthelot mixing rules are used in order to calculate the LJ interactions of dissimilar atoms. Universal Force Field (UFF) parameters are employed throughout the simulations (Rappe et al., 1992). In the case of CO_2 and N_2, electrostatic interactions described via Coulomb's potential are also taken into account in addition to dispersion interactions. CO_2 is modeled as a three-site rigid linear molecule with the charges located on each atom using EPM2 potential (Potoff and Siepmann, 2001). N_2 molecule is defined

with a three-site model with two sites located on two N atoms and one site is on the molecule's center of mass with partial point charges (Makrodimitris et al., 2001). Electrostatic charges on MOF atoms are reproduced from the study of Erucar et al. (2014) where charges of the MOF atoms are derived from density derived electrostatic and chemical (DDEC) method. Simulation results of the CO_2-MOF systems using DDEC method has already shown to agree well with the experimental results (Erucar et al., 2014). While cut-off distance is set as 13 Å for the LJ interactions, 25 Å is used for the electrostatic interactions. Periodic boundary conditions are always applied.

2x2x2 replica of the unit cell is used as a simulation box. 3×10^7 trial configurations are used in the GCMC simulations in total, where half of the moves are considered as equilibration, thus the other half is used for the data collection. In single component GCMC simulations, a move is defined as translation, creation/deletion, and rotation (in the case of CO_2 and N_2) of the particles. In the case of mixture simulations, on the other hand, an additional move of exchange of the particles are also attempted.

A good indication of the promising adsorbent materials is their high selectivity towards a gas specie. The adsorption selectivity is calculated using the equation below:

$$S_{ads}(i/j) = x_i/x_j \, y_i/y_j \qquad (1)$$

here x and y are the molar fractions of the adsorbed and gas phases of the species, respectively. For the mixture adsorption simulations CO_2/Xe and Xe/N_2 mixture compositions are set to 20/80 and 80/20, respectively.

3. Results and Discussion

Single component and mixture adsorption isotherms of CO_2 and Xe species as a function of bulk pressure at 298 K in considered MOFs are depicted in Figure 1. As a first observation, although in CECYOY and SUDBOI single component CO_2 adsorption is higher than the one observed for single component Xe, in ZUQPOQ pores of the nanoporous material attract CO_2 and Xe gas species as a similar manner leading similar adsorption amount for both gas species. At 10 bar of feed pressure, single component CO_2 adsorption data of CECYOY, SUDBOI, and ZUQPOQ are calculated as 10.90, 13.50, and 4 molecules/unitcell, respectively. Single component Xe uptake at 10 bar, on the other hand, are calculated as 8.45, 5.54, and 3.94 molecules/unitcell in CECYOY, SUDBOI, and ZUQPOQ, respectively. The gap between single component uptakes of CO_2 and Xe is more pronounced in the case of SUDBOI, where saturated CO_2 and Xe uptakes are 14.60 and 6.20 molecules/unitcell, respectively. While CECYOY and SUDBOI reach saturation of adsorption of the single component species at around 25 bar, in the case of ZUQPOQ CO_2 and Xe gas species reach saturation point at a lower pressure, around 4 bar.

Mixture gas adsorption simulation results reveal that both CO_2 and Xe adsorption are affected from each due to filling of the available adsorption sites by dissimilar specie. While CO_2 is interacting with the MOF adsorbents through electrostatic and dispersion interactions, its only dispersion type interaction in the case of Xe. Due to this reason, we observe that Xe adsorption is always suppressed by CO_2 adsorption for CO_2/Xe:20/80 mixture in considered MOFs.

We observe a sharp decrease in the CO_2 uptakes of the MOFs in the mixture case with respect to its single component adsorption amount. However, this decrease is less pronounced in the case of CECYOY, where at 10 bar mixture CO_2 adsorption amount is decreased to 6.60 molecules/unitcell. We observe even more significant decrease in the Xe adsorption amount for the case of mixture gas simulations in all considered MOFs. At 10 bar calculated Xe uptake values for the CO_2/Xe:20/80 mixture are 3.34, 0.36, and 1.30 molecules/unitcell in CECYOY, SUDBOI, and ZUQPOQ, respectively.

The significant decrease in the mixture Xe adsorption isotherms are attributed to the attractive electrostatic interactions between CO_2 and the MOF atoms resulting in occupation of the adsorption sites by the CO_2 molecules. Prevention of the Xe adsorption is more pronounced in the CECYOY and SUDBOI with respect to ZUQPOQ. We observe competition between electrostatic and dispersion interactions. Combination of electrostatic and dispersion interactions between CO_2 and MOF atoms outperform mixture Xe adsorption in the pores, yielding adsorption based separation of CO_2/Xe mixture.

N_2 and Xe mixture adsorption isotherm calculations are carried out using 20% and 80% composition of N_2 and Xe gases, respectively. Corresponding GCMC results are shown in Figure 2.
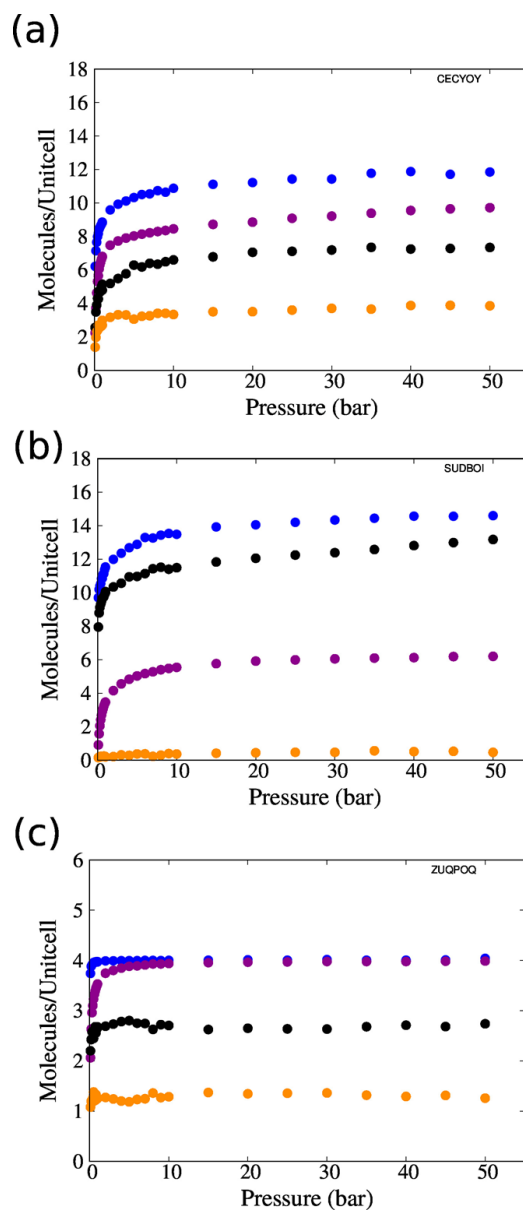
(a)

(b)

(c)

Figure 1. Single specie and mixture uptake data of CO_2/Xe in (a) CECYOY, (b)SUDBOI, and (c) ZUQPOQ carried out at 298 K. Xe and CO_2 compositions of the feed gas is set to 80% and 20%, respectively. Blue circles represent single component CO_2 uptake, purple ones depict single component Xe uptake, black circles show CO_2 uptake in the mixture, and orange ones depict Xe uptake in the CO_2/Xe:20/80 mixture.

As a general observation, for the single component gas specie adsorption, while Xe adsorption reaches saturation in the MOF pores at smaller pressure values, around 4 bar, in the case of N_2 adsorption, we observe

saturation at significantly high pressures, around 50 bar, for all the considered MOFs. Xe uptake of MOFs increases steeply at early pressure values.

Xe/N_2:80/20 mixture adsorption calculations reveal that, dispersion interactions between Xe and MOF atoms outperform N_2 adsorption in the pores. MOF pores are filled by Xe atoms, and negligibly low amount of N_2 molecules can find place on the adsorption sites. As it can be seen from Figure 2, while there is almost negligible change between the values of single component and mixture Xe adsorption, a sharp decrease is observed in the case of mixture N_2 with respect to its single component adsorption values.

In fact, N_2 adsorption is almost blocked by the Xe atoms in all the MOFs under consideration. Preferable adsorption of Xe atoms over N_2 have been also observed in the literature in other MOFs. For instance, Panter and Zarabadi-Poo (2018) studied Xe separation from air in several IRMOF materials and results always indicate selective adsorption of Xe over N_2 molecules. Zhong et al. (2016) investigated the Xe/N_2 adsorption-based separation of adsorption performance of nitrogen-doped porous Carbon material which shows exceptional Xe uptake over N_2.

Mixture N_2 adsorption preference of the considered MOFs shows the opposite behavior with respect to the mixture CO_2 adsorption considering preferable CO_2 adsorption in the MOFs. As in the case of CO_2, N_2 molecules are also interacting through electrostatic and dispersion interactions with the MOF pores.
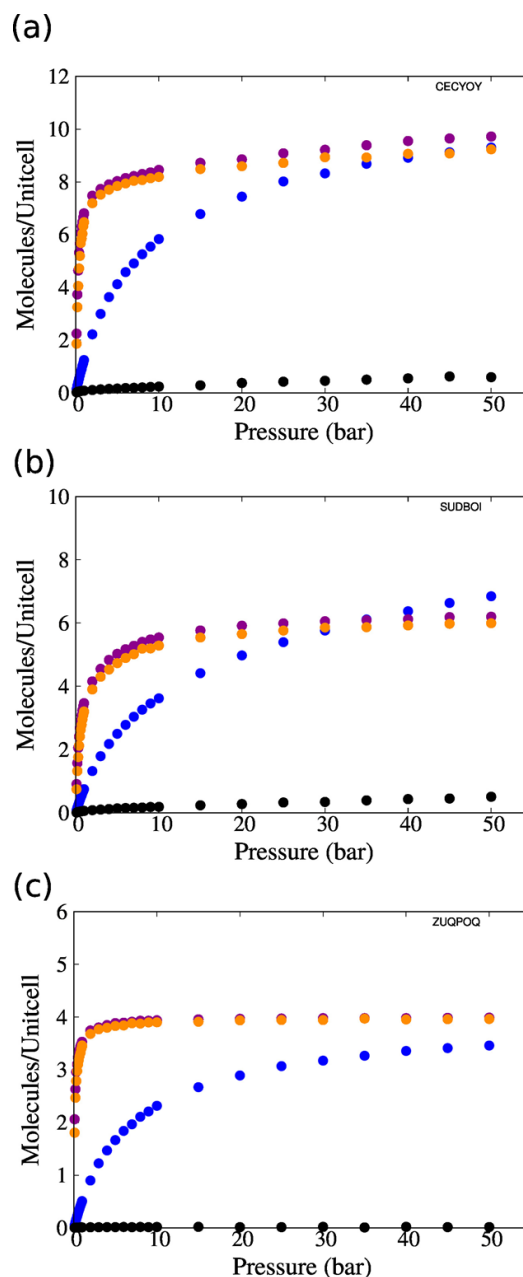

Figure 2. Single specie and mixture uptake data of Xe/N_2 in (a) CECYOY, (b)SUDBOI, and (c) ZUQPOQ carried out at 298 K. Xe and N_2 compositions of the feed gas is set to 80% and 20%, respectively. Blue circles represent single component N_2 uptake, purple ones depict single component Xe uptake, black circles show N_2 uptake in the mixture, and orange ones depict Xe uptake in the Xe/N_2:20/80 mixture.

To investigate the effects of electrostatics on the adsorption of mixture CO_2 and mixture N_2 species, we carry out GCMC analysis using CECYOY by turning-off electrostatic interactions. Figure 3 shows the adsorption isotherms of CO_2 and N_2 by turning on and off electrostatic interactions for CO_2/Xe and Xe/N_2 mixtures. As it can be seen from Figure 3, turning-off electrostatic interactions has insignificant effect on both mixture CO_2 and mixture N_2 adsorption amounts. This result suggest that dispersion type interaction is the key factor determining adsorption isotherms. Electrostatic interactions having small effect in modeling gas-MOF systems have been also discussed in the study of Erucar et al. [19], where turning-off electrostatics in modeling CO_2/CH_4, CO_2/N_2, and H_2/CO_2 adsorption and diffusion in MOFs can give similar results with the electrostatics-on scenario.
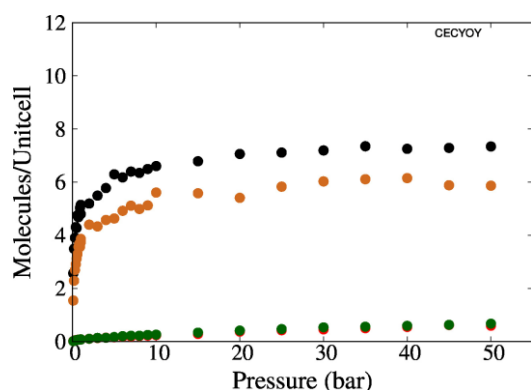

Figure 3. Effects of electrostatic interactions on mixture CO_2 and N_2 adsorption isotherms calculated for CECYOY. While black (brown) circles show electrostatic interactions on (off) calculations for CO_2, red (green) shows electrostatics on (off) calculations for N_2.

As it is clear from Figure 3, dispersion type interactions are playing determining role in mixture Xe and N_2 adsorption of considered MOFs. Energy force field parameters of the CO_2 and Xe are much higher than the one for N_2 which explains preferable adsorption of CO_2 or Xe adsorption over N_2. Considering larger adsorption of CO_2 with respect to Xe is,

instead, related with the steric hindrance affects. Van der Waals size of the Xe atom is larger than the one used for CO_2, which prevents further adsorption of Xe atom in the MOF pores.

The adsorption based separation performances of the considered MOF materials are further investigated by calculating their adsorption selectivities with respect to feed gas pressure, see Figure 4. While for the CO_2/Xe:20/80 mixture CO_2 is the mostly adsorbed specie, in the case of Xe/N_2:80/20 Xe adsorption is preferable. Thus, CO_2 and Xe adsorption selectivities of the MOFs are calculated for CO_2/Xe and Xe/N_2 mixtures, respectively.

As it can be seen from Figure 4(a), SUDBOI shows the highest CO_2 adsorption selectivity among the other MOFs. At 0.1 bar CO_2 adsorption selectivity is calculated as 205, and as pressure increases selectivity decreases to 110 in SUDBOI. In the case of CECYOY and ZUQPOQ, on the other hand, selectivity values are around 10 and we observe negligible change in the selectivities as the pressure increases.

For the Xe/N_2:20/80 mixture, see Figure 4(b), ZUQPOQ shows the largest Xe selectivity, where at 0.1 bar Xe selectivity is calculated as 68 and as pressure increases it decreases to 55. Xe selectivity values of CECYOY and SUDBOI are similar to each other, and at higher pressures Xe selectivities are decreased to 5 for both MOFs.
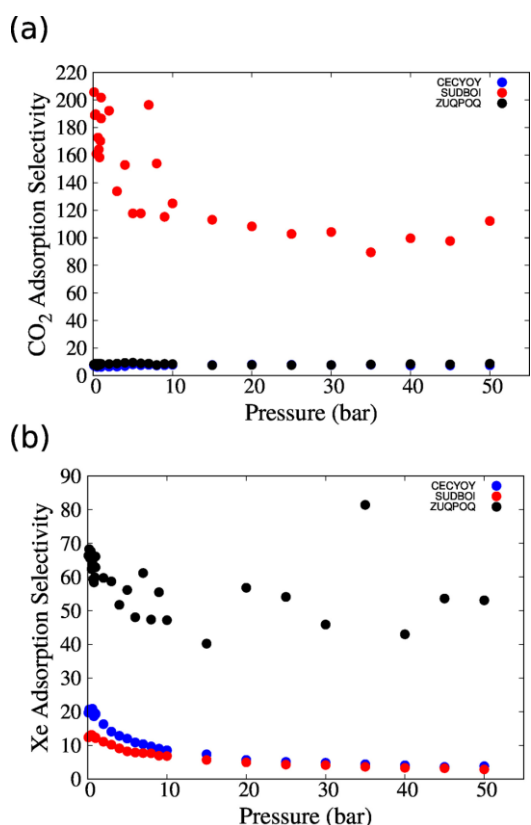
(a)

(b)

Figure 4. (a) CO_2 and (b) Xe adsorption selectivity with respect to feed pressure for CO_2/Xe and Xe/N_2 mixtures, respectively. Selectivity values calculated for CECYOY, SUDBOI, and ZUQPOQ are depicted using blue, red, and black circles, respectively.

4. Conclusion

We theoretically investigate adsorption-based anesthetic Xe recovery from the exhale gas for clinical industry by taking advantage of MOFs. We perform GCMC simulations to calculate adsorption isotherms of single component and binary mixtures of CO_2, Xe, and N_2. To mimic the anesthetic exhale gas composition, we determine the gas mixture compositions as $CO_2/Xe:20/80$ and $Xe/N_2:80/20$. Equilibrium adsorption amounts of the gas species and adsorption selectivities are determined for the MOFs, namely CECYOY, SUDBOI, and ZUQPOQ. Results reveal that while more CO_2 adsorption

is preferred for the CO_2/Xe mixture, Xe adsorption is more facilitated for the Xe/N_2 mixture in the considered MOFs. These results are attributed to the higher energy parameter of the Xe atom with respect to N_2 which leads to enhanced dispersion type interactions between MOF pores and Xe atoms, thus preference of Xe adsorption over N_2. In the case of CO_2/Xe mixture, on the other hand, size parameter of CO_2 is smaller than Xe. Thus, CO_2 molecules fill the pores easier than Xe atoms which are prevented due to steric hindrance effects.

Adsorption selectivity calculations reveal that while SUDBOI shows significantly large CO_2 adsorption selectivity for CO_2/Xe, ZUQPOQ has the largest Xe selectivity for the $Xe/N2$ mixture.

Our results suggest that while SUDBOI is ideal candidate for CO_2 separation from CO_2/Xe, ZUQPOQ can be considered as promising candidate for Xe separation from Xe/N_2 mixture. However, Xe recovery scenarios are different in these MOFs, since SUDBOI separates Xe by facilitated CO_2 adsorption over Xe, and ZUQPOQ separates Xe by facilitated Xe adsorption over N_2. Thus, two step procedure for recovering anesthetic Xe can be proposed, such as firstly CO_2 can be separated from the exhale gas mixture by CO_2 adsorption in SUDBOI, then Xe/N_2 gas mixture can be separated by Xe adsorption in ZUQPOQ in the second step.

Our research can proceed in many directions. We simulate the adsorption based separation of binary anesthetic gas mixtures. Thus, simulating ternary mixtures of $CO_2/Xe/N_2$ is highly motivated. Besides, it is known that an extent of H_2O and O_2 are also present in the anesthetic exhale gas mixtures. The effects of all these gas species on Xe recovery

performances of MOFs are open questions that should be addressed. The results of this study with the possible extensions can provide a cheaper solution for Xe recovery in the clinical industry using the advantages of MOFs.

Acknowledgments

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