ChemPor 2023

14th International Chemical and Biological Engineering Conference

Book of Abstracts

Instituto Politécnico de Bragança | September 12-15

ORDEM DOS ENGENHEIROS

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This volume contains the extended abstracts presented at the 14th International Chemical and Biological Engineering Conference (CHEMPOR 2023), held in Bragança - Portugal, from the 12th to the 15th of September, 2023.

Instituto Politécnico de Bragança & Ordem dos Engenheiros

14th International Chemical and Biological Engineering Conference

(CHEMPOR-2023)

Book of Abstracts

Edited by:

Ana Maria Alves Queiroz da Silva

António Manuel Coelho Lino Peres

António Manuel Esteves Ribeiro

Maria Filomena Filipe Barreiro

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INSTITUTO POLITÉCNICO DE BRAGANÇA

Title

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Editors

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Programme

Time		Tuesday 12	Wednesday 13			Thursday 14			Friday 15		
08:00	09:00		*Registration*								
09:00	09:15										
09:15	09:30		**Plenary lecture 1**			**Plenary lecture 3**			**Plenary lecture 5**		
09:30	09:45		Jarka Glassey - **ADG**			Raquel Aires-Barros - **ADG**			Rafael Luque - **ADG**		
09:45	10:00										
Session-Room			**S1-AAM**	**S1-ADG**	**S1-AP**	**S4-AAM**	**S4-ADG**	**S4-AP**	**S7-AAM**	**S7-ADG**	**S7-AP**
10:00	10:15		O EE-01	O BS-01	O RS-01	O BT-04	O MS-13	O RS-09	O BS-07	O RS-12	O BT-10
10:15	10:30		O EE-02		O RS-02	O BT-05	O MS-02	O RS-10	O BS-02	O RS-13	O BT-11
10:30	10:45		O EE-03	O BS-03	O RS-03	O BT-06	O MS-03	O RS-11	O BS-09	O RS-14	O BT-12
10:45	11:00		**Poster session 1**			**Poster session 2**			*Coffee-break*		
11:00	11:15		*Coffee-break Topics - EE IA MS and RS*			*Coffee-break Topics - BS BT and IM*					
11:15	11:30		**Keynote 1** - Juan F. Rodríguez - **AAM**			**Keynote 3** - Maria José Ferreira - **AAM**			**Keynote 5** - José Palomar - **AAM**		
11:30	11:45		**Keynote 2** - Luís Madeira - **ADG**			**Keynote 4** - Miguel Cerqueira - **ADG**			**Keynote 6** - Mara Freire - **ADG**		
Session-Room			**S2-AAM**	**S2-ADG**	**S2-AP**	**S5-AAM**	**S5-ADG**	**S5-AP**	**S8-AAM**	**S8-ADG**	**S8-AP**
11:45	12:00		O IM-01	O EE-04	O BT-01	O BT-07	O BS-04	O IM-04	O RS-15		O BS-10
12:00	12:15		O IM-02	O EE-05	O BT-02	O BT-08	O BS-05	O IM-05	O RS-16	O IM-10	O BS-11
12:15	12:30		O IM-03	O EE-06	O BT-03	O BT-09	O BS-06	O IM-06	O RS-17	O IM-11	O BS-12
12:30	14:00		*Lunch*								
Session-Room									**S9-AAM**	**S9-ADG**	**S9-AP**
14:00	14:15								O IA - 05	O RS-18	O BT-13
14:15	14:30		**Plenary lecture 2**			**Plenary lecture 4**			O IA - 06	O RS-19	O BT-14
14:30	14:45		Joaquim Henrique Teles - **ADG**			Margarida Costa Gomes - **ADG**			O IA - 07	O RS-20	O BT-15
14:45	15:00									O RS-21	O BT-16
Session-Room			**S3-AAM**	**S3-ADG**	**S3-AP**	**S6-AAM**	**S6-ADG**	**S6-AP**			
15:00	15:15		Sysadvance	Paralab	O EE-07	O IA - 01	O MS-04	O EE-13	O EE-19	O MS-10	O IM-12
15:15	15:30		O RS-04	Bondalti	O EE-08	O IA - 02	O MS-05	O EE-14	O EE-20	O MS-11	O IM-13
15:30	15:45		O RS-05	Bruker	O EE-09	O IA - 03	O MS-06	O EE-15	O EE-21		O IM-14
15:45	16:00		O RS-06	Prio	O EE-10	O IA - 04	O MS-07	O EE-16	**Awards ceremony - ADG**		
16:00	16:15	*Registration*	O RS-07	Cires	O EE-11	O IM-07	O MS-08	O EE-17	**CHEMPOR-2026**		
16:15	16:30		O RS-08	Hovione	O EE-12	O IM-08	O MS-09	O EE-18	**Closing session**		
16:30	16:45		**Poster session 1**			**Poster session 2**					
16:45	17:00		*Coffee-break*			*Coffee-break*					
17:00	17:15	**Opening ceremony - TMB**	*Topics - EE IA MS and RS*			*Topics - BS BT and IM*					
17:15	17:30	**Opening lecture**									
17:30	17:45	Jorge Calado									
17:45	18:00	**Honor session**									
18:00	19:00	Alírio Rodrigues				***Social program***					
19:00	19:30										
19:30	23:00					***Conference dinner***					

BS	Biorefinery and Sustainability
BT	Biotechnology
EE	Energy and Environment
IA	Industrial Applications
IM	Innovative Materials
MS	Modeling, Synthesis and Integration of Chemical Processes
RS	Reaction and Separation Processes

AAM	Auditório Alcínio Miguel
ADG	Auditório Dionísio Gonçalves
AP	Auditório Pequeno
TMB	Teatro Municipal de Bragança

Influence of [emim][Tf_2N] in PES/SAPO-34 mixed matrix membranes for gas separation

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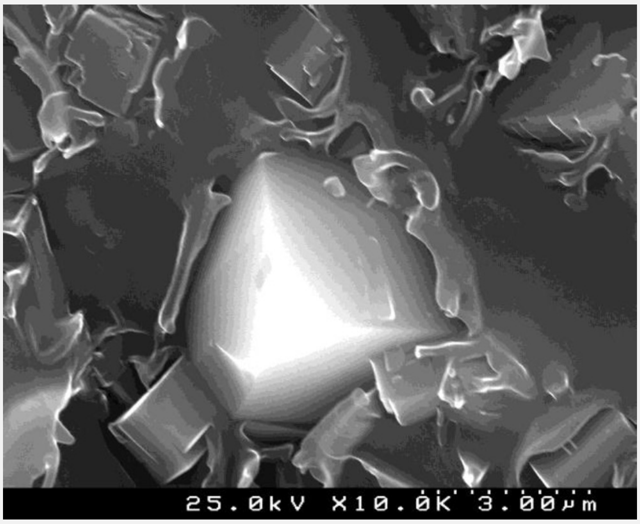

Mixed matrix membranes (MMM) are heavily studied and the main concern by researchers is the difficulty to obtain a high selectivity membrane with low defects, mainly interfacial voids due to the poor interaction between polymer matrix and filler. The functionalization of zeolite surface in Poly-EtherSulphone (PES)/Silico-AluminoPhosphate-34 (SAPO-34) led to membranes with higher compatibility. Recently, the use of ionic liquids in the particles surface to improve the gas permeability and separation efficiency has presented advanced results. The aim of this work is to compare the separation efficiency of CO_2 and N_2 in permeance and selectivity criteria. The use of the ionic liquid (IL) [emim][Tf_2N] showed an increase in selectivity and in CO_2 permeance due to promoting a better separation of the dispersant in the polymeric matrix when compared to a film with the same composition without the IL treatment.

Introduction

The silicoaluminophosphates-34 (SAPO-34) appears as one of the main materials in mixed matrix membranes (MMM) for gas separation because of its pore size (0.38nm) is near the kinetic diameter of gases like H_2 (0.29nm), CO_2 (0.33nm), N_2 (0.36nm), CO (0.37nm) and CH_4 (0.38nm). Those materials have been dispersed in a polymeric matrix aiming to obtain membranes with more thermal stability and more selectivity than polymeric membranes, which are more permeable than inorganic membranes. Although PSA, TSA and cryogenic distillation are mostly used industrially in CO_2 separation, the use of MMM with zeolites and other silicate derivatives as constituents of MMM in gas separation, provides lower energy consumption, is modulable and can be connected to traditional processes, besides showing permeability and selectivity above the Robeson upper limit [1-5]. The surface functionalization of inorganic solids arises to improve the zeolite-polymer matrix interaction. ILs are proposed to improve the interaction between those components, increasing the membrane separation performance [6-10].

Materials and Methods

SAPO-34 sample was synthesized using a gel with the molar composition 1.0Al_2O_3; 1.0P_2O_5; 0.6SiO_2; 1.5Morpholine; 0.5Tetraethylammonium hydroxide (TEAOH); 70H_2O. The zeolite was prepared using a dry-gel methodology with 1:1 mass ratio of dry mass/water, heated at 200 °C for 24 h. The produced mixture was then centrifuged, washed, dried at 105 °C in an oven and calcined at 560 °C for 8 h. The samples were characterized via Powder X-Ray Diffraction (PXRD), Dynamic Light Scattering (DLS) and N_2 adsorption and desorption.

20%w/w PES/SAPO-34 membranes were prepared by adding the zeolite in stirring N-Methyl-2-pyrrolidone (NMP) for 1 h and in ultrasonic bath for 4 h. Then a small amount of PES was added to the NMP/SAPO-34 solution and mixed for 1 h at 80 °C. The remaining PES was added and mixed for 3 h at 80 °C, and the solution was stirred overnight at room temperature. The solutions were degassed for 4 h in ultrasonic bath and casted with a knife of 0.3 mm, dried at 80 °C for 2 h and at 200 °C for 20 h under vacuum. The 20%w/w PES/SAPO-34/[emim][Tf_2N] membranes synthesis followed the same procedure using 20%w/w of IL. The samples were characterized by scanning electron microscopy (SEM). Gas permeation experiments were conducted using pure gases to determine their permeability and diffusivity coefficients, and the results were compared to each other in a permeability unit called Barrer ($10^{-10}\, cm^3_{STP} \cdot cm/cm^2 \cdot s \cdot cmHg$). A schematic of the permeation system is shown in Figure 1 and the permeabilities were obtained according to Eq. 1. The ideal selectivity results (α_{ab}) are represented by the ratio between the permeability (P) of two pure gases, a and b, respectively, measured separately under the same conditions, in the same membrane to evaluate the separation performance, as presented in Eq. 2.

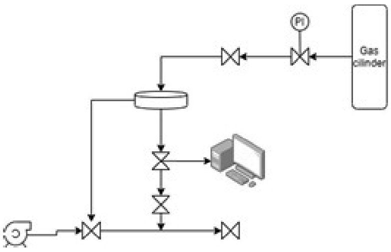

Figure 1. Schematic of the permeation system.

$$P_i = \frac{V_s l}{T_{AMB}\Delta p}\frac{T_{STP}}{p_{STP}A}\frac{dp}{dt} \quad (1)$$

$$\alpha_{a/b} = \frac{P_a}{P_b} \quad (2)$$

Results and discussions

Pure SAPO-34 was synthetized for a reaction time of 24 h using the methodology described and named JS1. The XRD pattern was compared to a standard one. The average particle size obtained was around 0.2 µm, as presented in Figure 3. The

N_2 adsorption-desorption isotherms in Figure 2 exhibited a type I isotherm which is characteristic of microporous structure. The textural properties show that the material presented a high BET area (S_{BET}) and V_{mic} which are comparable to those in literature.

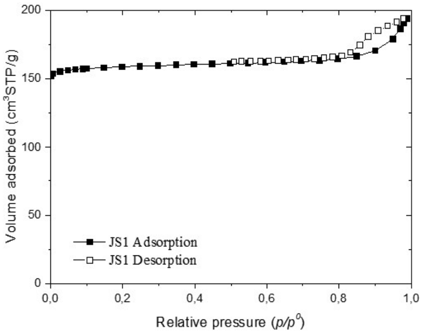

Figure 2. N_2 adsorption-desorption isotherm of JS1.

Table 1. Textural properties of JS1.

Sample	
S_{BET} (m^2 g^{-1})	464
V_{mic} (mm^3 g^{-1})	0.25

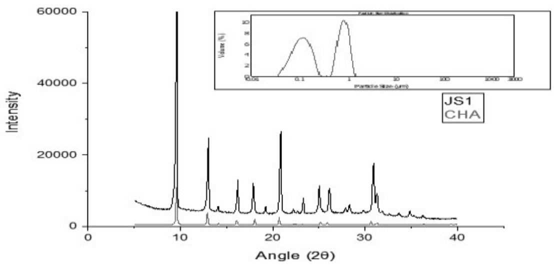

Figure 3. XRD and DLS for JS1 sample.

Fig 4a presents the SEM analysis of PES/SAPO-34 membrane with an agglomeration of crystal along the polymeric matrix. Figure 4b presents the SEM analysis of the PES/SAPO-34/[emim][Tf$_2$N] membrane with a more disperse crystals in the polymeric matrix. Figure 5 shows that the agglomeration of crystals in (a) presents voids between particles without selectivity, which causes an increase in permeation of all gases with a selectivity reduction. However, the more dispersed crystals presented in (b) are mainly due the use of IL, which helped to involve the crystals reducing agglomeration. This can be noted in CO_2 and N_2 permeability and separation selectivity as presented in the Table 2. The PES/SAPO-34/[emim][Tf$_2$N] membrane presented a higher CO_2 permeability and higher selectivity when compared to PES/SAPO-34 membrane, showing that the incorporation of [emim][Tf$_2$N] improved the separation performance.

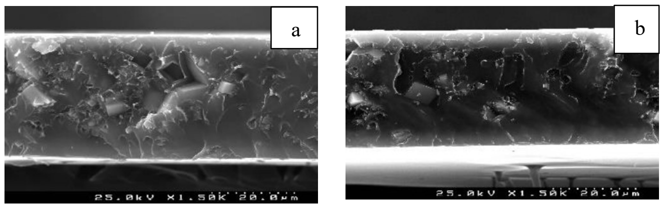

Figure 4. Cross-section of (a)PES/SAPO-34 and (b)PES/SAPO-34/[emim][Tf$_2$N] membranes.

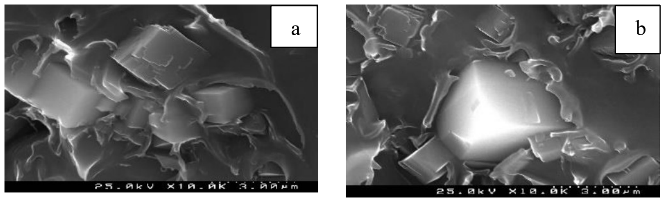

Figure 5. Zoom in particle distribution for (a)PES/SAPO-34 and (b)PES/SAPO-34/[emim][Tf$_2$N] membranes.

Table 2. Separation performance of PES/SAPO-34 and PES/SAPO-34/[emim][Tf$_2$N] membranes.

Sample	P_{CO2} (Barrer)	P_{N2} (Barrer)	$\alpha_{CO2/N2}$
PES/SAPO-34	0,83	0,04	18,83
PES/SAPO-34/[emim][Tf$_2$N]	2,11	0,05	39,44

Conclusions

The methodology for nano-sized SAPO01-34 preparation was stablished as well as the solid with the desired characteristics was used as filler in MMM. The use of the ionic liquid [emim][Tf2N] promoted an increase in separation performance in PES/SAPO-34 membrane due an increase in the dispersion of the crystals in the polymeric matrix, promoting an improvement in the CO_2 permeation and selectivity of the membranes. Other ionic liquids and deep eutectic solvents are planned to be tested and compared, as a more eco-friendly and less expensive alternatives, in order to understand the effects of those in the separation performance of PES/SAPO-34.

Acknowledgements

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