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Modeling N2/CH4 Flow in Separation Process using a Zeolite Membrane: A CFD Approach

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Abstract

In this work, the main objective is to study, through Computational Fluid Dynamics (CFD), the process of separating N2/CH4 gases using a zeolite membrane. The membrane permeance and geometry are included in the simulations based on values observed in experiments. Through this work, our goal is to develop a robust and reliable numerical methodology to simulate the N2/CH4 gas separation process. Computational simulations are performed using the finite volume method, through OpenFOAM, a free and open-source software widely used in industry and academia. The equations of mass conservation, momentum balance, energy conservation, and mass concentration are solved at each time step. The preliminary results presented here illustrate the flow within the separation module and demonstrate that the developed methodology is capable of simulating the gas separation process.

Introduction

In recent years, research on natural gas separation using zeolite membranes has attracted significant attention [4]. This research can be pursued through experimental and theoretical paths. However, experimental methods often incur high costs, longer duration, and lack easy visualization of internal flow. To overcome these challenges, numerical simulations offer a promising alternative, enabling flexible parameter adjustments, cost reduction, and comprehensive analysis of process dynamics [2, 5]. In this study, our objective is to develop a robust and reliable methodology for simulating gas flow through the separation process facilitated by zeolite membranes, with a particular focus on CH4/N2 separation.

Methodology

The equations of mass conservation, momentum balance, energy conservation, and mass concentration [1, 2], which model the gas flow in the addressed problem, are numerically solved in this work using the finite volume method with the OpenFOAM 11 software (openfoam.org). In the simulations, the flow is considered laminar and the simulations are transient. Figure 1 illustrates the geometry and mesh (with 168983 cells), where the membrane measures 10 cm in length and has a diameter of 5 mm. The system comprises one inlet (feed), one outlet for the retentate, and one outlet for the permeate (with the latter being blocked). Gas enters the feed with a mass concentration of 0.5 for CH4 and 0.5 for N2, at a flow rate of 10^{-5} kg/s. The pressure at the permeate outlet is maintained at 10^{5} Pa, while the pressure at the retentate outlet is 4 x 10^{5} Pa. The feed temperature is 293 K and the walls are insulated. The membrane used in this preliminar investigation, a SSZ-13, has a N2 permeance of 2.38 x 10^{-8} kg m^{-2} s^{-1} Pa^{-1} and a CH4 permeance of 1.01 x 10^{-9} kg m^{-2} s^{-1} Pa^{-1} [3]. The final time is 15 s and the time-step is defined in order to get a Courant number of 0.1 .

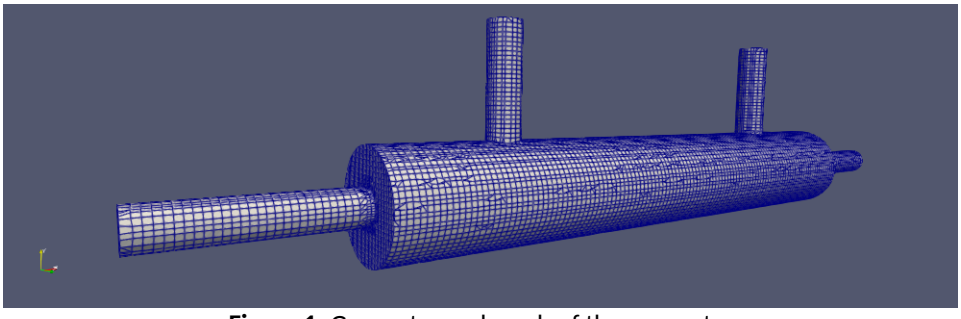

Figure 1: Geometry and mesh of the apparatus.

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Results and Conclusions

The passage of gas through the membrane affects the concentration of CH4 and N2 along the flow. Figures 2 and 3 show the mass fraction of CH4 in the apparatus. At the inlet, the fraction is 0.5, while the fraction is 0.604 at the retentate outlet. The increase in fraction occurs due to higher permeance of N2 through the membrane. There is also a significant variation in the CH4 fraction in the transverse direction to the flow. In addition to the observed jump due to the presence of the membrane, there is also a significant variation in mass fraction within the retentate, with a minimum value observed at the center of the geometry. The effect of this transverse gradient of mass fraction on the gas separation outcome is not yet well understood, and is one of the points we intend to explore in future work.

In this work, a methodology for simulating the behavior of a gas during the separation process by zeolite membrane was implemented and it is being tested. The methodology was validated with experimental results [1] and utilized to understand the flow of a gas composed of CH4 and N2 under different permeance conditions. A significant concentration gradient was observed in the transverse direction to the flow, which may directly impact gas separation. As future work, the authors will analyze different flow rates, permeances and other membrane configurations, such as disc and hollow-fiber.

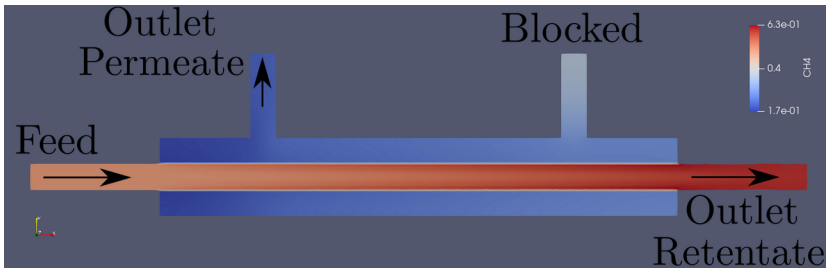

Figure 2: Mass fraction of CH4 in the apparatus.

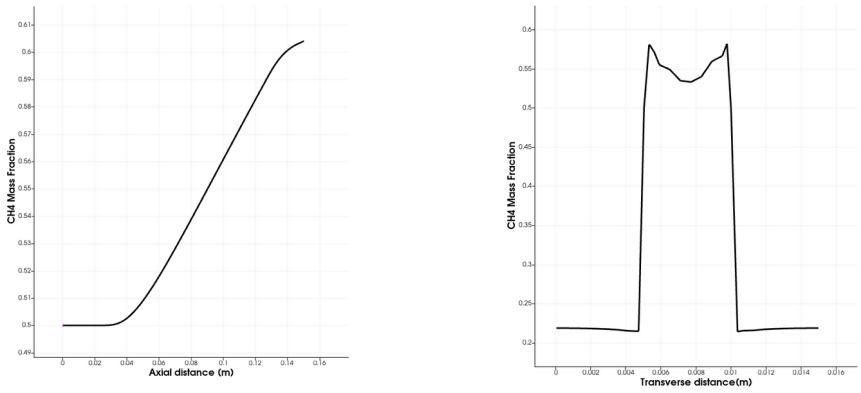

Figure 3: Axial and transverse mass fraction of CH4.

References

[1] dos Anjos, S. C. J., B. G. Pimenta, B. E. Leite, A. P. Rosa and A. M. A. Silva, “Simulação numérica de membranas de zeólita para a separação de N2/CH4,” unpublished.

[2] Haddadi, B., Jordan, C., Miltner, M. and Harasek, M. “Membrane modeling using CFD: Combined evaluation of mass transfer and geometrical influences in 1D and 3D,” Journal of Membrane Science, 563, 199–209 (2017).

[3] Li, Y., S. He, C. Shu, X. Li, B. Liu, R. Zhou and Z. Lai, “A facile approach to synthesize SSZ-13 membranes with ultrahigh N2 permeances for efficient N2/CH4 separations,” Journal of Membrane Science, 632, 119349 (2021).

[4] Silva, A. M. A, A. Carolina, B. D. Faria, C. D. Lima, D. D. Athayde, E. Paulo, G. Magalhães, L. Fernando, D. S. Lima, R. Nunes, D. Souza, S. Lucas and N. D. S. Mohallem, “Review of zeolite membranes for natural gas processing and treatment : State of the art and future perspectives,” Gas Science and Engineering, 117, 205056, 2023.

[5] Qadir, S., A. Hussain and M. Ahsan, “A computational fluid dynamics approach for the modeling of gas separation in membrane modules,” Processes, 7, 7 (2019).