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Kawachale, Nikhil; Kumar, Ashwani; Kirpalani, Deepak

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Nikhil Kawachale¹
Ashwani Kumar¹
Deepak M. Kirpalani¹

¹Institute for Chemical
Process and Environmental
Technology, National Research
Council of Canada, Ottawa,
Canada.

Research Article

Numerical Investigation of Hydrocarbon Enrichment of Process Gas Mixtures by Permeation through Polymeric Membranes

In membrane-based gaseous separations, a consensus on the distribution of the components of the permeate stream in the immediate membrane vicinity has yet to be reached and the possibility of an underestimation of selective gas permeance due to lack of gas mixing on the permeate side exists. In this work, a numerical study of the permeation of ethylene and propylene in their binary mixtures with nitrogen through a composite poly(dimethylsiloxane) coated polysulfone membrane was performed. Continuity and momentum equations, along with gas compressibility and permeance properties for individual species of the gas mixture, were introduced into a comprehensive computational fluid dynamics (CFD) model. Simulation results showed that irrespective of the stage-cut, gases with higher selectivity were well mixed in the vicinity of the membrane on the permeate side.

Keywords: CFD, Hydrocarbons, Nitrogen, Separation, Silicone-coated membrane

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1 Introduction

The vent streams from many manufacturing processes in polymer and petrochemical industries, fuel storage and painting operations often contain a large amount of volatile organic compounds (VOC). In order to recover VOCs and to minimize emissions, most conventional methods such as adsorption and low temperature condensation have been unsatisfactory, particularly for lower VOC concentrations [1]. Large volumes of VOC and nitrogen-containing streams are encountered in resin degassing and nitrogen blanketing operations in the polymer and petroleum processing industries. After the initial recovery of hydrocarbons by condensation, a lean mixture of VOC and nitrogen is either vented to the atmosphere or flared. In both cases, the practice not only represents a loss of hydrocarbons and energy but also contributes to the emission of greenhouse gases (GHG). Implementation of an energy efficient process to recover hydrocarbons and reuse the nitrogen would lead to significant savings of hydrocarbons and reduction in emission of GHGs. Due to its favorable process economics and ease of operation, membrane technology provides

an attractive alternative for separating VOCs and nitrogen mixtures.

Previous research has focused on developing an understanding of the permeation, sorption and diffusion effects of VOCs on membranes coated with rubbery polymers [2]. Among the rubbery polymers, poly(dimethylsiloxane) (PDMS) was reported to be a solubility selective polymer that is more permeable to condensable vapors than noncondensable gases [3]. It is well-known that the performances of a pressure-driven membrane separation depends on both the membrane characteristics and the transport phenomena occurring adjacent to the feed and permeate side of the membrane. The design of the membrane module is of fundamental importance in achieving higher efficiency during separation. In most separation applications, mathematical models have been developed to predict process performance for design and optimization. General models based on permeation have been reported for co-current and counter-current pressure driven gas separation processes [4, 5]. In addition, the Hagen-Poiseuille equation is generally applied to predict the pressure drop and determine concentration polarization on the permeate side of the hollow-fiber membrane [6]. However, most models assume ideal gas flow or the existence of well mixed gas species on both the feed and permeate sides of the membrane, which may affect the estimated membrane performance. Furthermore, the mass transfer along with fluid dynamics in membrane separation is typically represented by coupling film theory with empirical correlations that yield the mass-transfer coefficients or the

Correspondence: Dr. A. Kumar (ashwani.kumar@nrc-cnrc.gc.ca), Institute for Chemical Process and Environmental Technology, National Research Council of Canada M-12 Montreal Road Campus, Ottawa, Ontario, K1A 0R6, Canada.

Sherwood number as a function of the Reynolds and Schmidt numbers [7]. However, such empirical correlations were originally developed for impermeable interfaces and have been directly applied to permeable membrane systems without modification. An implementation of these models to membrane may ignore the effects of the permeation rate on the velocity and concentration profiles in the fluid phase contiguous to the membrane surface. Moreover, in the case of gas separation systems, it has always been difficult to predict the mixing of the interacting gas species on the permeate side [3].

Computational fluid dynamics (CFD) together with mass transfer modeling could depict actual fluid dynamics and solute concentration distribution in complex membrane cell geometries. During the past decade, hydrodynamic studies with interacting species were performed using CFD simulations to enable visualization of species and streamlines of flow. Koukou et al. [8] performed detailed CFD simulation to study concentration polarization in pressure-driven gas separation processes with selective membrane and outlined a framework for modeling the separation process. An application and validation of a CFD model for pressure-driven membrane separation of incompressible mixtures that focuses mainly on selective component rejection with concentration polarization on the membrane surface was reported by Wiley and Fletcher [9]. However, the reported results were constrained since the membrane was treated as an impermeable wall with no concentration build-up and the mass transport across the membrane was neglected. This might lead to inaccurate prediction of the overall hydrodynamics and separation phenomena. To overcome this problem, Wiley and Fletcher [10] conducted a two-dimensional (2D) CFD simulation that involved predicting concentration polarization by applying a wall concentration gradient at the impermeable interface. In addition, Geraldes et al. [11] developed a numerical model to predict laminar flow hydrodynamics and mass transfer of aqueous solutions in the feed channel of spiral-wound and plate-and-frame systems. The utilization of CFD simulation to predict the concentration polarization profile and mass-transfer coefficient for liquid or incompressible mixture separation over a range of operating conditions in a membrane channel was reported by Ahmed et al. [12]. They used a sodium chloride and water solution in the feed channel to analyze the hydrodynamics of the fluid adjacent to the membrane. The only gas mixture separation study performed using CFD was reported by Takaba and Nakao [13]. They modeled the selective extraction of H_2 from a H_2/CO mixture through a ceramic membrane and analyzed the CFD results to determine a separation factor and flux for comparison with conventional plug flow calculations. Plug flow modeling was found to be suitable only for low permeability conditions.

However, a comprehensive computational study that considers both high and low stage-cuts and mass flow rates to depict the actual conditions in the immediate membrane environs has not yet been performed. This has been partially due to the absence of detailed and reliable experimental permeance data for process design. This has further limited the development of a realistic picture of mass flows and permeating gas concentrations in the immediate membrane vicinity. In the present study, a CFD model that represents the underlying

flow dynamics and species permeation with a focus on gaining a better understanding of the mixing of binary gas species on the permeate side of the membrane, is applied in conjunction with recently reported experimental permeance data [3].

2 CFD Methodology and Numerical Solutions

2.1 Scope of CFD

CFD modeling, coupled with the gas transport could be considered as a detailed mathematical procedure to study the hydrocarbon separation from a binary gas mixture with the objective of visualizing the flow and gas mixing inside the membrane cell. The coupled CFD approach can model the mass flow through a mathematical coupling of the species continuity and momentum in a compressible solver with defined permeances. The permeation flux, total mass flow and mass fractions of different components can be taken into account within the solution of these governing equations. The probable effects of feed concentrations together with membrane stage-cuts on a desired separation can also be included within a model. The integration of permeation properties across a membrane along with the gas mixture dynamics in a CFD environment was found to present a significant challenge [14]. The effect of spacers on the flow hydrodynamics of the feed channel is known and several CFD studies entailing membrane based liquid-liquid separations are available [7, 10, 12]. However, the incorporation of permeation properties in CFD codes to predict the mixing of gases in the immediate membrane vicinity of the permeate side has not been accounted for to date.

2.2 Simulation Conditions

Jiang and Kumar [3] reported studies on binary gas mixtures, e.g., ethylene (C_2H_4)/nitrogen (N_2) and propylene (C_3H_6)/nitrogen (N_2), at constant feed pressure and concentrations. The simulation studies presented in this work were validated with reported permeance values [3]. A schematic of the membrane module used by Jiang and Kumar [3] is shown in Fig. 1. The studied membrane comprised of a highly microporous polysulfone support coated with a 0.2 μm thick PDMS layer. The flat sheet membrane used in a stainless steel module (SEPA® CF Membrane Cell) had an effective area of 0.0135 m^2 . The experimental conditions were maintained at steady state with laminar flows, $Re < 225$, and ambient temperature, 22 $^{\circ}C^{(1)}$.

2.3 Governing Equations

The governing equations, based on the physical principles of continuity, momentum conservation and solute conservation, are shown in Eqs. (1–5).

1) List of symbols at the end of the paper.

– Equation for conservation of mass (continuity):

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho \omega)}{\partial z} = 0 \quad (1)$$

– Equation of Momentum (Navier-Stokes):

In the x -direction:

$$\rho \left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + \omega \frac{\partial u}{\partial z} \right) = - \left(\frac{\partial P}{\partial x} \right) + \left(\frac{\partial}{\partial x} \mu \left(\frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \mu \left(\frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \mu \left(\frac{\partial u}{\partial z} \right) \right) \quad (2)$$

In the y -direction:

$$\rho \left(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + \omega \frac{\partial v}{\partial z} \right) = - \left(\frac{\partial P}{\partial y} \right) + \left(\frac{\partial}{\partial x} \mu \left(\frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \mu \left(\frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial z} \mu \left(\frac{\partial v}{\partial z} \right) \right) \quad (3)$$

In the z -direction:

$$\rho \left(u \frac{\partial \omega}{\partial x} + v \frac{\partial \omega}{\partial y} + \omega \frac{\partial \omega}{\partial z} \right) = - \left(\frac{\partial P}{\partial z} \right) + \left(\frac{\partial}{\partial x} \mu \left(\frac{\partial \omega}{\partial x} \right) + \frac{\partial}{\partial y} \mu \left(\frac{\partial \omega}{\partial y} \right) + \frac{\partial}{\partial z} \mu \left(\frac{\partial \omega}{\partial z} \right) \right) \quad (4)$$

– Equation of solute concentration (conservation):

$$\begin{aligned} & \rho \left(u \frac{\partial(C_A)}{\partial x} + v \frac{\partial(C_A)}{\partial y} + \omega \frac{\partial(C_A)}{\partial z} \right) \\ &= \left(\frac{\partial}{\partial x} \rho D_{AB} \left(\frac{\partial C_A}{\partial x} \right) + \frac{\partial}{\partial y} \rho D_{AB} \left(\frac{\partial C_A}{\partial y} \right) + \frac{\partial}{\partial z} \rho D_{AB} \left(\frac{\partial C_A}{\partial z} \right) \right) \end{aligned} \quad (5)$$

Eqs. (1–5) were solved for a three-dimensional (3D) domain for laminar flow with steady-state operation to examine the gas flow characteristics and concentration profiles of the species. For the detailed 2D simulations, the ' z ' terms in Eqs. (1–5) were omitted. Non-slip boundary conditions at the wall surface and variation in solute concentration were also included in the compressible solver. In addition, based on the empirical data, plasticization effects were neglected and the partitioning of hydrocarbon from the bulk feed to the membrane was not considered to be mass transfer limiting.

Figure 1. Schematic of VOC separation module.

2.4 Domain Generation

Computations were performed on a grid that was generated by using the meshing software GAMBIT® 2.2. The dimensions of the computational domain were identical with that of the SEPA® CF Membrane Cell used in the experimental work by Jiang and Kumar [3]. Structured meshing was performed to divide the flow domain into subdomains and quadrilaterals cells, and the discretized governing equations were solved inside each cell. The continuity and momentum equations across the common interfaces between two subdomains, the feed and the permeate side, were solved to visualize fluid flow in the entire domain. The membrane cell computational geometry consisted of a mass flow inlet, boundary for introducing the feed mixture and two pressure outlets for retentate and permeate flows. The membrane in the domain was defined as shadowed wall, while all other edges represented the barriers of the remaining cell geometry. The computational grid consisted of 13 'Mass-Flow-Inlet' edge cells with 19 'Pressure-Outlet' edge cells and 1460 'Wall' edge cells on either side of the membrane. In total, 27740 quadrilateral cells in the fluid zone were used to mesh the computational domain of length, $L = 0.146$ m and height, $H = 0.018$ m. Grid refinement was performed to achieve grid independence by analyzing the concentration gradient within the geometrical domain.

2.5 Solution Method and Solver Settings

Model development and simulations were performed in CFD software (FLUENT® 6.2). All the functions required to compute a solution and to display the results in this software were accessible either through an interactive interface or by including user-defined functions. In the present simulation, the gas mixture properties were defined before executing the simulation loop. Operating parameters, such as mass flow rate, pressure and species concentrations were obtained and implemented as boundary conditions from empirical data for the two different binary mixtures [3]. The simulations were performed using steady-laminar flow conditions at ambient temperature. The discretization of the governing equations was performed using a segregated compressible flow solver in which each governing equation is solved separately. Given that the velocities obtained earlier might not satisfy the continuity equation locally, pressure-velocity coupling was used to obtain the necessary corrections to the pressure and velocity fields along with the face mass fluxes, such that the continuity equation is satisfied.

The Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) formulation was set as a part of a pressure-velocity coupling algorithm [15]. In order to update the velocity field, the Navier-Stokes equations were solved using current values for cell nodal pressures and face mass fluxes. The discrete velocities and pressures were stored in cell centers by a nonstaggered system, which consisted of cells and faces. The fluid properties were updated based on the previous iterations or given initial values. The convergence criteria for the continuity and velocity parameters were fixed at 0.001 %. A higher convergence criterion, i.e., $1.0 \cdot 10^{-7}$ %, was set for hydrocarbons

to offer sufficient iterations for complete convergence between the boundary and the interior mesh grid. In order to obtain a stable solution, the under relaxation factors, which limit the influence of the previous iteration over the present one were fixed to 0.3 for the pressure, 1 for density, 0.7 for the momentum and 1 for species. Lower values of the under relaxation factors were selected for pressure and momentum to prevent oscillating solutions [16]. The pressure was set to 'Pressure Straggering Option' (PRESTO!) and momentum, density and mass fractions were set to 'Second Order Upwind' discretization schemes for more accurate results. The 'Aggressive Advanced Multigrid' (AMG) scheme had been applied to accelerate the convergence of the solver by computing corrections on a series of coarse grid levels. The AMG cycle type for the coupled equations involving pressure, momentum and species concentration was set to fixed 'F-Cycle' as a recursive procedure. In addition, the 'Biconjugate Gradient Stabilized Method' (BCGSTAB) was employed to solve nonsymmetrical linear systems to avoid the frequent irregular convergence patterns [16].

2.6 User Defined Function (UDF)

As demonstrated in Fig. 2, the 'User Defined Function' (UDF) was compiled and then hooked to the solver during simulation, and thus, linked to the iterative procedure to perform simulations. Subsequently, after each iteration, solver data was updated repetitively by the UDF. Transport of gas across the membrane was achieved using a series of user-defined functions in FLUENT® software. Membrane modeling was addressed by incorporating permeabilities and mass fluxes as a UDF written in 'C code' that virtually overrides the 'Wall' parameters in the solver as the solution proceeds. The issue of hydraulic jump across the membrane was resolved by patching the cells from the upper and lower zones with two different values of initial pressures. The 'Define Profile' macro was used in parallel with the adjacent cell index to link the relationship between the hydrodynamics and the membrane transport phenomena. Changes in the fluid flow adjacent to the membrane interface were accounted for by the UDF with the prediction of new parameters for the membrane wall along with the shadow side. In addition, the UDF updated the solver data with new parameters at the membrane wall. The source and sink terms in the UDF were calculated by using the simple relationship between the linear flux and the driving force for the gas diffusion in the membrane as shown in Eq. (6):

$$J_i = -D_i \frac{dC_i}{dN} \quad (6)$$

In case of gas transport through the membrane, this general phenomenological equation is commonly known as Fick's first law of diffusion that can be further simplified as:

$$J_i = \frac{P_i}{l} (p_{fi} - p_{pi}) \quad (7)$$

The term $\frac{P_i}{l}$ in Eq. (7) can be defined as permeance, which is a pressure and thickness normalized flux. In the existing UDF, the above equations were incorporated as:

Figure 2. Solution strategy for comprehensive hydrocarbon separation model.

$$J_i = \frac{P_i}{l} \frac{\vec{A}}{v} MW_i (p_{fi} - p_{pi}) \quad (8)$$

The mass flux was calculated for all the species in the mixture, on both sides of the membrane as source and sink terms. Moreover, the 'Jacobian' of the source and sink terms had been considered in the UDF to achieve enhanced solution stabilization. The stability and convergence of the mass source were improved since the source terms were linearized by using the derivatives of the same. The developed comprehensive model accounts for pressure variation from the feed to the permeate side in the membrane module with pressure-density corrections by using the ideal gas law for the gas mixtures.

2.7 Preliminary Simulations

The simulations involving the actual geometry of the SEPA cell were first run with a 3D grid. Figs. 3a) and 3b) shows the concentration profiles for C_2H_4/N_2 and C_3H_6/N_2 binary mixtures at a virtual surface below the membrane, $H = 4.57 \cdot 10^{-4}$ m, for low stage-cuts values. It can be seen from Figs. 3a) and 3b) that the concentration profile varies along the channel length, L , while the concentration changes across the channel width, W , were not significant. The minor discrepancy in the concen-

Figure 3. Mass fraction of hydrocarbons across the virtual surface below the membrane, $H = 4.57 \cdot 10^{-4}$ m, at a low stage-cut: (a) C_2H_4 ($Y_{C_2H_4}$), $\sigma = 0.16$, and (b) C_3H_6 ($Y_{C_3H_6}$), $\sigma = 0.12$.

trations across the cell width close to the channel wall could be due to wall effects. Moreover, at any given point across the channel width, the simulation results would be same as in the case of 2D geometry. Therefore, for computational economy without sacrificing a better understanding, all subsequent simulations were performed in a 2D environment.

3 Results and Discussion

The mixing of permeating gases was studied numerically over a range of hydrocarbon feed concentrations and stage-cut values in binary gas mixtures. Computational models were found

to converge to a steady solution in 60 s. CFD simulation results were compared with experimentally measured boundary parameters [3]. It was found that the numerical predictions are in good agreement with empirical data for flow rates and species concentrations. This established the effectiveness of applying CFD-based modeling approaches for studying the internal flow and species distribution in gas separation membrane systems.

In order to examine the hydrocarbon concentration near the membrane surface, virtual edges were generated numerically at a distance of one computational cell ($9.2 \cdot 10^{-5}$ m) on both sides of the membrane length. Hydrocarbon concentrations and mass flow rates were computed on the virtual edges (Isosurfaces) to determine the extent of mixing in the immediate vicinity of the membrane. Results for the permeation of C_2H_4/N_2 and C_3H_6/N_2 through PDMS membrane mixtures are shown in Figs. 4–9.

Fig. 4a) shows the mass fraction of C_2H_4 for different stage-cuts at a virtual edge above the membrane length, $H = 6.44 \cdot 10^{-4}$ m. It is clear from Fig. 4a) that at low initial feed mass fractions of hydrocarbon, the concentration change across the membrane is very low. However, the change increases with an increase in stage-cut values. In addition, at higher hydrocarbon feed concentrations, it is noted that the rate of change of concentration on the feed side of the membrane along the channel length is higher than that of the lower feed hydrocarbon concentration. Fig. 4b) shows the mass fraction of C_2H_4 as a function of channel length at a virtual edge below the membrane, $H = 4.57 \cdot 10^{-4}$ m, over a range of stage-cuts. It is evident from

Fig. 4b) that the permeate side C_2H_4 concentration in the vicinity of the membrane increases with a decrease in feed concentration. As the permeating mass was accumulating below the membrane before leaving the cell, the concentration profiles on the permeate side complement those on the feed side, to some extent. Although, membrane stage-cuts influence the separation behavior, the concentration profile formed near the feed or permeate side of the membrane has a higher dependency on the feed hydrocarbon concentration than the stage-cut, i.e., $\sigma = 0.17$ and $\sigma = 0.20$ in Figs. 4a) and 4b), respectively. The total permeate mass flow profiles for C_2H_4/N_2 separation across the permeate surface of the membrane at $H = 5.50 \cdot 10^{-4}$ m over the range of stage-cuts, is shown in Fig. 5.

Figure 4. Mass fraction of C_2H_4 ($Y_{C_2H_4}$) for different stage-cuts, σ across the virtual edge: (a) above the membrane, $H = 6.44 \cdot 10^{-4}$ m, and (b) below the membrane, $H = 4.57 \cdot 10^{-4}$ m.

Figure 5. Total permeate mass flow rate of C_2H_4/N_2 (Q_p) over the range of stage-cuts, σ , across the membrane, $H = 5.50 \cdot 10^{-4}$ m.

Figure 6. Overlaid plot of contours of mass fraction of C_2H_4 ($Y_{C_2H_4}$) and gas mixture velocity vectors in the feed, retentate and permeate sections of computational domain at a low stage-cut, $\sigma = 0.16$.

Figure 7. Mass fraction of C_3H_6 ($Y_{C_3H_6}$) for different stage-cuts, σ , across the virtual edge: a) above the membrane, $H = 6.44 \cdot 10^{-4}$ m, and (b) below the membrane, $H = 4.57 \cdot 10^{-4}$ m.

Figure 8. Total permeate mass flow rate of C_3H_6/N_2 (Q_p) over the range of stage-cuts, σ , across the membrane, $H = 5.50 \cdot 10^{-4}$ m.

Figure 9. Overlaid plot of contours of mass fraction of C_3H_6 ($Y_{C_3H_6}$) and gas mixture velocity vectors in the feed, retentate and permeate sections of computational domain at low stage-cut, $\sigma = 0.12$.

The mass flow rate confirms a higher dependency of the concentration profile on the feed hydrocarbon concentration than on the stage-cut, i.e., $\sigma = 0.17$ and $\sigma = 0.20$ in Fig. 5, and shows the expected gradient in mass flow rate across the channel length.

In order to depict the mixing behavior and flow profile, the contour plots of the inlet and outlet regimes, where the entrance and exit effects were expected to be prominent, are illustrated in Fig. 6. The change in parameters observed in the section between the inlet and outlet sections of the computational domain was observed to be rather uniform, and thus, was not shown here. The C_2H_4 concentrations overlaid with velocity vectors converged from empirical data with a low stage-cut, $\sigma = 0.16$, is demonstrated at a feed section, $L = 0\text{--}0.017$ m, together with the retentate and permeate sections of cell geometry, $L = 0.129\text{--}0.146$ m. It can be observed from Fig. 6 that a marginal decrease in feed velocity leads to a minor build up of feed concentration near the entrance. As a result, the concentration

polarization combined with high operating pressures encountered during gas separation result in higher hydrocarbon permeation near the feed section. In addition, with an increase in feed velocity, the permeation rates decrease in accordance with the empirical results [3]. It is clearly evident from the contours in Fig. 6 that the hydrocarbon and nitrogen are well mixed in the immediate vicinity of the membrane on the permeate side. Moreover, in the case of higher stage-cut values, the species were observed to be more evenly distributed in the immediate vicinity of the membrane.

Feed and permeate concentrations at varying stage-cuts for binary mixtures of propylene and nitrogen are shown in Figs. 7a) and 7b). It is obvious from Figs. 7a) and 7b) that the patterns of the concentration profiles observed for C_3H_6 were similar to those for C_2H_4 . However, it appears that the concentration profiles are dependent on the feed hydrocarbon concentration rather than the stage-cut, unlike the cases of C_2H_4/N_2 separation. Fig. 8 shows the total permeate mass flow profiles for C_3H_6/N_2 separation across the permeate surface of the membrane over the range of stage-cuts. Although, the mass flow profiles of C_3H_6/N_2 separation depends more on hydrocarbon concentration than on stage-cut, the mass flows for C_3H_6/N_2 separation are comparable to those for C_2H_4/N_2 separation. Furthermore, the trends observed in the overlaid contour plots of C_3H_6/N_2 separation for low stage-cut, $\sigma = 0.12$, as shown in Fig. 9 are similar to those of C_2H_4/N_2 . Minor differences regarding the vector magnitudes and concentration distribution could be due to different experimental conditions and mixture properties. Consequently, at any given solute concentration or stage-cut in the feed, the species on the permeate side are well distributed. Hence, it can be inferred that the concentration of solute in the feed combined with stage-cut affects the concentration profile of well mixed gases on the permeate side in the vicinity of the membrane.

4 Conclusions

A comprehensive computational study that couples continuity and momentum equations with Fick's law of gas diffusion was developed to illustrate the mixing behavior of the gas species in the immediate membrane environs. The results from the 2D simulation environment adopted in this work were found to be in agreement with the 3D model indicating that the concentration and flux variation along the width of the membrane was insignificant. The proposed CFD model was coupled with the solution-diffusion equation and validated with experimental data. Over the wide range of membrane stage-cuts and feed concentrations, it was concluded that the species in the immediate membrane vicinity were found to be well mixed. The model also suggests the need for including both stage-cut and feed concentrations in determining the performance of gas separation membrane systems. There is a potential to extend the simulation procedure by introducing variable permeances to obtain an improved understanding of the permeation of gases through membranes. The application of the described CFD methodology forms a framework for numerical studies in gas separation and can be further extended to other membrane systems with different geometries and gas mixtures.

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Symbols used

$\vec{A}$	[m ²]	area magnitude vector
C	[wt %]	concentration
D	[m ² s ⁻¹]	diffusion coefficient
H	[m]	cell height
J	[molm ⁻² s ⁻¹]	flux
l	[μm]	membrane thickness
L	[m]	cell length
MW	[-]	molecular weight
N	[-]	space coordinate normal for component i
p	[Pa]	partial pressure
P	[Pa]	pressure
P	[m ² s ⁻¹ Pa ⁻¹]	permeability
Re	[-]	Reynolds number
Q	[kgs ⁻¹]	mass flow
u	[ms ⁻¹]	velocity in x -direction
v	[m ³]	volume of cell
W	[m]	cell width
x	[-]	x -coordinate
y	[-]	y -coordinate
Y	[-]	mass fraction
z	[-]	z -coordinate

Greek symbols

μ	[kgm ⁻¹ s ⁻¹]	viscosity
v	[ms ⁻¹]	velocity in y -direction

ω	[ms ⁻¹]	velocity in z -direction
ρ	[kgm ⁻³]	density
σ	[-]	stage-cut

Subscripts

AB	components A and B
f	feed side
i	species
p	permeate side

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