Pure oxygen separation from air using dual-phase SDC-SCFZ disc membrane: A modelling approach

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Abstract. Novel Ce0.8Sm0.2O1.9-SrCo0.4Fe0.55Zr0.05O3-δ (SDC-SCFZ) disc membranes consist of 25 wt.% SDC fluorite ionic conducting phase and 75 wt.% SCFZ perovskite mixed conducting phase, which is more promising than perovskite oxide SCFZ single-phase membrane in terms of the oxygen permeation flux. This work features a modelling approach to simulate the oxygen permeation fluxes of the SDC-SCFZ membrane. Simplified model equations from the Zhu model and Xu-Thomson model based on the limiting cases of surface exchange reactions and bulk diffusion are compared. The Zhu model is found to be more applicable for the membranes with overall good correlation and low sum of squared error. Furthermore, modelling studies revealed that the oxygen transport is limited by surface exchange reactions from 700 to 850 °C and a mixture of both limiting cases above 850 up to 950 °C. It is concluded that the membranes exhibit high oxygen permeation flux of up to 2×10⁻⁶ m³ s⁻¹ cm⁻² at 950 °C with P air of 5 atm and P O₂ of 0.005 atm. The optimum range of operating conditions of the membrane are found to be at 950 °C with minimum P air of 1 atm and P O₂ lower than 0.025 atm.

1. Introduction

Mixed ionic-electronic conducting (MIEC) membrane is extensively utilised as an oxygen separation pathway alternative to pressure swing adsorption and cryogenic distillation [1]. This is due to its numerous advantages such as lower capital and operational costs, lower energy consumption, simpler process engineering and better scalability [1]. The membrane can attain up to 99.99 % oxygen product purity and 100 % oxygen selectivity when operated at elevated temperature (above 700 °C). The central theme of research activities for oxygen separation using MIEC membranes is primarily centred on achieving high oxygen permeation flux and good chemical stability of materials as well as exploring engineering methods and designs to improve the performance of the membrane. Different techniques such as engineering approaches, which are exemplified by mixing of ionic conducting phase and electronic conducting phase, geometry modification, internal and external short circuits, and modification of membrane surface or materials development approaches, which are represented by chemical doping have been widely investigated to boost the oxygen permeation flux of the membrane [2].

SrCo0.4Fe0.55Zr0.05O3-δ (SCFZ) is a perovskite-type oxygen permeable membrane, which is prepared by doping of fluorite-related structure ZrO2 into perovskite-related structure SrCo0.8Fe0.2O3-δ (SCF) [3]. The doping of Zr into SCF enhances the structural stability in the presence of CO2 and H2O-containing atmosphere, making it possible to retain its perovskite structure even after operating at 700 °C for 10
hours [4]. This is ascribed to the reduction of the oxygen vacancy concentration by the Zr$^{4+}$ metal ion substitution [5]. Since the SCFZ membrane can retain its structure in the presence of CO$_2$ and H$_2$O, ambient air can be directly utilised as feed. Although the doping of Zr into SCFZ membrane may cause the oxygen flux of the membrane to be reduced, the flux is found to be more stable than SCF membrane over long time operation [6]. The doping of 9 wt.% of ZrO$_2$ in SCFZ membrane has produced 4.04×10$^{-7}$ mol s$^{-1}$ cm$^{-2}$ of stable oxygen permeation flux at 900 °C over a 240 hours period [7].

Ce$_{0.8}$Sm$_{0.2}$O$_{1.9}$-SrCo$_{0.4}$Fe$_{0.55}$Zr$_{0.05}$O$_{3-\delta}$ (SDC-SCFZ) disc membrane, which consists of 25 wt.% Ce$_{0.8}$Sm$_{0.2}$O$_{1.9}$ (SDC) fluorite ionic conducting phase and 75 wt.% SrCo$_{0.4}$Fe$_{0.55}$Zr$_{0.05}$O$_{3-\delta}$ (SCFZ) perovskite mixed conducting phase, is found to be more promising than perovskite oxide SCFZ single-phase membrane in terms of oxygen permeation flux and structural stability. The high ionic diffusivity and structural stability of SDC fluorite (as the ionic conducting phase) [1] and the stable and good oxygen permeation in SCFZ perovskite (as the mixed conducting phase) [3] are expected to endow SDC-SCFZ dual-phase membranes with good oxygen permeation performance [7].

Modelling plays a significant role towards describing oxygen permeation behaviour. Using small sets of experimental data, modelling provides insights on dominant variables as well as predicts close to actual experimental results and behaviour from the simulation [8]. Thus, modelling can contribute better knowledge and understanding towards development of membranes. Thus far, numerous oxygen permeation models had been developed so that the diffusion kinetics, oxygen exchange kinetics and degradation mechanism for MIEC membranes can be well understood [9]. Among the available oxygen permeation models, the Zhu and Xu-Thomson models have been widely applied to various MIEC membranes. The Zhu model is a simple permeation model that was introduced by Zhu et al. [10] based on the theoretical analysis of electrochemical processes within the membrane interfaces as well as within the membrane bulk. Another oxygen permeation model by Xu and Thomson [11] was introduced based on the surface reaction model from Lin, Wang and Han [12], whereby the oxygen permeation is driven by the oxygen chemical potential gradient and the surface reactions are not influenced by the membrane interface thickness.

Thus far, a suitable oxygen permeation model that conforms well to the permeation data of SDC-SCFZ disc membrane and can determine the oxygen permeation behaviour has yet to be identified. Therefore, this work features the determination of a suitable oxygen permeation model for SDC-SCFZ disc membrane through a modelling approach using the Zhu and Xu-Thomson models. This paper determines the limiting case of SDC-SCFZ disc membrane in each temperature range using simplified model equations based on the surface exchange or bulk diffusion limited cases, which constitutes a simple approach to replace the entire model for simulation while still attaining accurate results. Furthermore, this paper provides new insights on the performance of SDC-SCFZ disc membrane through a parametric study.

2. Methodology

2.1 Source of experimental data

SCFZ powders were synthesised through solid-state reaction, as reported elsewhere [14]. SrCO$_3$ (99.0%), Co$_2$O$_3$ (99.0%), Fe$_2$O$_3$ (99.0%), and ZrO$_2$ (99.0%) were stoichiometrically mixed and milled for 5 hours followed by drying for 24 hours. Then the mixed powders were calcinated in air at 950 °C for 4 hours with ramping and cooling rates of 3 °C min$^{-1}$. The calcined SCFZ powders were mixed with Sm$_{0.2}$Ce$_{0.8}$O$_{1.925}$ (SDC, fuelcellmaterials, SDC20-TX) powders using SDC:SCFZ weight ratio of 25:75 in an agate mortar. The weight ratio of 25:75 was selected in this work based on the highest oxygen permeation fluxes reported among other SDC-SCFZ dual-phase membranes [14]. The ground powder mixture was ball milled in ethanol for 5 hours followed by drying for at least 24 hours. The powders were then pressed into disks of 0.95 cm diameter using a mould before they were sintered in air at 1200 °C for 5 hours to obtain dense membranes with a thickness of 0.06 cm.

The oxygen permeation performance of the membrane was evaluated from 950 to 700 °C at decreasing intervals of 50 °C. At each temperature, feed side oxygen partial pressure ($P_{O_2}^f$) was varied
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from 0.7 to 0.2 \text{atm} at decreasing intervals of 0.1 \text{atm}. Helium gas was introduced to sweep the permeated oxygen and the permeate side oxygen partial pressure \((P_{O_2}^{\text{P}})\) was recorded. The oxygen permeation flux was determined from the measured oxygen concentration and outlet flow rate.

2.2 Modelling for oxygen permeation tests

The Zhu model and Xu-Thomson model equations are simplified according to the surface exchange reactions and bulk diffusion limited cases to simplify the flux simulation of SDC-SCFZ disc membrane. equation 1 and 2 represent the oxygen fluxes calculated using the Zhu model while equation 3 and 4 represent oxygen fluxes calculated using the Xu-Thomson model. \(J_{O_2,\text{ex}} (\text{mol s}^{-1} \text{ cm}^{-2})\) represents the fluxes calculated based on surface exchange reaction limited case while \(J_{O_2,\text{diff}} (\text{mol s}^{-1} \text{ cm}^{-2})\) represents the fluxes calculated based on bulk diffusion limited case. All the simplified model equations are adapted from Shubnikova et al. [13].

\[
J_{O_2,\text{ex}} = \gamma(T)_{\text{surface ex}} \frac{(P_{O_2}^f)^{\frac{1}{2}} (P_{O_2}^P)^{\frac{1}{2}}}{(k_{f} p_{O_2}^f)^{\frac{1}{2}} + (k_{p} p_{O_2}^P)^{\frac{1}{2}}} \ln \left( \frac{P_{O_2}^p}{P_{O_2}^f} \right)
\]

\[
J_{O_2,\text{diff}} = \gamma(T)_{\text{bulk}} \ln \left( \frac{P_{O_2}^p}{P_{O_2}^f} \right)
\]

\[
J_{O_2,\text{ex}} = \gamma(T)_{\text{surface ex}} \frac{p_{O_2}^f p_{O_2}^P}{p_{O_2}^f + p_{O_2}^P}
\]

\[
J_{O_2,\text{diff}} = \gamma(T)_{\text{bulk}} \frac{p_{O_2}^P}{p_{O_2}^f + p_{O_2}^P}
\]

\[k_1 (\text{mol s}^{-1} \text{ cm}^{-2})\] is the rate constant corresponding to surface transport on the feed side on the membrane whereas \(k_2 (\text{mol s}^{-1} \text{ cm}^{-2})\) is the rate constant corresponding to surface transport on the permeate side on the membrane. \(C\) is the oxygen ion concentration (\text{mol cm}^{-3}), \(D\) is the bulk diffusion coefficient (\text{cm}^{2} \text{s}^{-1}) while \(h\) is the membrane thickness (cm). \(k_r\) and \(k_f\) are reverse (desorption) surface exchange rate constants (\text{mol s}^{-1} \text{ cm}^{-2}) and forward (adsorption) surface exchange rate constants (\text{cm atm}^{-0.5} \text{ s}^{-1}), respectively. \(P_{O_2}^f\) and \(P_{O_2}^P\), each with a unit of \text{atm}, are the feed and permeate side oxygen partial pressure, respectively. \(\gamma(T)\) is a temperature-dependent parameter that governs the oxygen transport depending on the limiting case of either bulk diffusion or surface exchange limited.

3. Results and discussion

3.1 Preliminary results

The model parameters in each limiting case of the Zhu and Xu-Thomson models are determined using MATLAB, the results of which are displayed in tables 1 to 4 along with the corresponding resultant coefficient of determination \((R^2)\) and sum of squared error (SSE) at each temperature point.
Table 1. Regressed oxygen permeation parameters for surface exchange reaction limited case using Zhu model.

| Temperature (°C) | Model parameter $k_1$ ($mol \ s^{-1} \ cm^{-2}$) | Model parameter $k_2$ ($mol \ s^{-1} \ cm^{-2}$) | $R^2$ | SSE |
|------------------|-----------------------------------------------|-----------------------------------------------|-------|-----|
| 950              | $3.800 \times 10^{12}$                        | $9.262 \times 10^{6}$                        | 0.845 | $1.526 \times 10^{-14}$ |
| 900              | $5.059 \times 10^{10}$                        | $7.169 \times 10^{6}$                        | 0.988 | $9.907 \times 10^{-16}$ |
| 850              | $1.879 \times 10^{6}$                         | $8.452 \times 10^{6}$                        | 0.998 | $1.042 \times 10^{-16}$ |
| 800              | $6.457 \times 10^{-7}$                        | $9.149 \times 10^{6}$                        | 0.980 | $3.662 \times 10^{-16}$ |
| 750              | $3.803 \times 10^{-7}$                        | $1.067 \times 10^{-5}$                       | 0.990 | $1.023 \times 10^{-16}$ |
| 700              | $2.526 \times 10^{-7}$                        | $1.888 \times 10^{10}$                       | 0.875 | $8.707 \times 10^{-16}$ |

Table 2. Regressed oxygen permeation parameters for bulk diffusion limited case using Zhu model.

| Temperature (°C) | Model parameter $\gamma$, $b_{ss}$ ($mol \ s^{-1} \ cm^{-2}$) | $R^2$ | SSE |
|------------------|---------------------------------------------------------------|-------|-----|
| 950              | $3.495 \times 10^{-7}$                                       | 0.882 | $1.163 \times 10^{-14}$ |
| 900              | $2.427 \times 10^{-7}$                                       | 0.703 | $2.454 \times 10^{-14}$ |
| 850              | $1.354 \times 10^{-7}$                                       | 0.398 | $3.316 \times 10^{-14}$ |
| 800              | $7.518 \times 10^{-8}$                                       | 0.295 | $1.282 \times 10^{-14}$ |
| 750              | $5.147 \times 10^{-8}$                                       | 0.161 | $8.252 \times 10^{-15}$ |
| 700              | $4.240 \times 10^{-8}$                                       | 0.081 | $6.376 \times 10^{-15}$ |

Table 3. Regressed oxygen permeation parameters for surface exchange reaction limited case using Xu-Thomson model.

| Temperature (°C) | Model parameter $\gamma$, $s_{asa}$ ($mol \ s^{-1} \ cm^{-2}$) | $R^2$ | SSE |
|------------------|----------------------------------------------------------------|-------|-----|
| 950              | $1.641 \times 10^{6}$                                        | 0.748 | $2.476 \times 10^{-14}$ |
| 900              | $1.164 \times 10^{6}$                                        | 0.533 | $3.865 \times 10^{-14}$ |
| 850              | $6.741 \times 10^{7}$                                        | 0.263 | $4.058 \times 10^{-14}$ |
| 800              | $3.762 \times 10^{7}$                                        | 0.190 | $1.475 \times 10^{-14}$ |
| 750              | $2.604 \times 10^{7}$                                        | 0.100 | $8.859 \times 10^{-15}$ |
| 700              | $2.133 \times 10^{7}$                                        | 0.050 | $6.592 \times 10^{-15}$ |
Table 4. Regressed oxygen permeation parameters for bulk diffusion limited case using Xu-Thomson model.

| Temperature (°C) | $\gamma(T),_{bulk}$ (mol atm$^{0.5}$ cm$^{-2}$ s$^{-1}$) | $R^2$    | SSE        |
|-----------------|-----------------------------------|----------|-----------|
| 950             | $1.982 \times 10^{-7}$            | -0.773   | $1.744 \times 10^{-13}$ |
| 900             | $1.257 \times 10^{-7}$            | -1.151   | $1.779 \times 10^{-13}$ |
| 850             | $6.055 \times 10^{-8}$            | -1.454   | $1.352 \times 10^{-13}$ |
| 800             | $3.253 \times 10^{-8}$            | -1.858   | $5.200 \times 10^{-14}$ |
| 750             | $2.115 \times 10^{-8}$            | -2.190   | $3.140 \times 10^{-14}$ |
| 700             | $1.747 \times 10^{-8}$            | -2.394   | $2.355 \times 10^{-14}$ |

3.2. Determination of SDC-SCFZ disc membrane’s oxygen permeation model

Based on the $R^2$ from preliminary results, the Zhu model exhibits good correlation between the modelled and experimental results for the surface exchange limited case given that the $R^2$ is greater than 0.8 between 700 and 950 °C (table 1), which exhibits relatively better correlation than the Xu-Thomson model (table 3). For the bulk diffusion limited case, the Zhu model only shows good correlation at 900 and 950 °C (table 2) while the Xu-Thomson model exhibits poor model behaviour given the negative $R^2$ which is attained from constraining the regressed model parameters to produce only positive values (table 4). Therefore, the oxygen transport according to the Zhu model is assumed to be limited by surface exchange reactions between 700 and 850 °C. The oxygen transport above 850 up to 950 °C is assumed to be limited by a mixture of both limiting cases as $R^2$ for the bulk diffusion case is relatively high compared to the other temperatures. However, the distribution of the two limiting cases cannot be accurately determined. To incorporate both limiting cases, a single equation (equation 5) was developed based on the aforementioned equations 1 and 2 used in this work. For the Xu-Thomson model, oxygen transport is assumed to be limited by surface exchange reactions from 700 to 950 °C. Therefore, equation 3 and the parameters from table 3 will be utilised for the Xu-Thomson model.

The model parameters of the Zhu model as well as $R^2$ and SSE for 900 and 950 °C are regressed from equation 5 based on the assumptions for mixed limiting case whereas the parameters between 700 and 850 °C are adapted from table 1 based on the assumptions of surface exchange limited case. The final Zhu model parameters used in this work are displayed in table 5. The large value of $k_2$ at above 900 °C in table 5 can be attributed to the larger influence of bulk diffusion.

Figure 1 exhibits a comparison of the linearised fluxes modelled using the Zhu and Xu-Thomson models. The modelled oxygen permeation fluxes calculated from the Zhu model have a good correlation with the experimental data based on figure 1(a) and also according to the high $R^2$ and low SSE in Table 5. From figure 1(b), the modelled oxygen permeation fluxes calculated using the Xu-Thomson model exhibit a bad correlation with experimental results. This together with low $R^2$ and high SSE attained in table 3 as compared to table 5 indicate a bad fitting and high error with the experimental data. Overall, the Zhu model produces better correlation than the Xu-Thomson model for dual-phase SDC-SCFZ disc membrane and will be utilised in the subsequent sections.

$$J = \gamma(T),_{surface} \cdot \left[ \frac{4P_{O2}^{0.5}P_{O2}^{0.5}}{4\gamma(T),_{bulk} + k_1 k_2 + 4k_2 k_1 P_{O2}^{0.5} + 4P_{O2}^{0.5}} \cdot \frac{k_1 k_2}{k_1 + k_2} \cdot \frac{k_1 k_2}{k_1 + k_2} \cdot \frac{\ln \frac{P_{O2}^{0.5}}{P_{O2}^{0.5}}}{\ln \frac{P_{O2}^{0.5}}{P_{O2}^{0.5}}} \right]$$

$$\gamma(T),_{surface} = \frac{1}{4} (k_1 k_2)^{1/2}$$

$$\gamma(T),_{bulk} = \frac{CD}{4h}$$

(5)
Table 5. Regressed oxygen permeation parameter for Zhu model.

| Temperature (°C) | $k_1$ (mol s$^{-1}$ cm$^{-2}$) | $k_2$ (mol s$^{-1}$ cm$^{-2}$) | $Y(\tau)$,bulk (mol s$^{-1}$ cm$^{-2}$) | $R^2$  | SSE  |
|-----------------|-------------------------------|-------------------------------|-------------------------------------|-------|------|
| 950             | 1.308×10$^{-4}$               | 1.492×10$^{-11}$              | 3.495×10$^{-7}$                     | 0.880 | 1.182×10$^{-14}$ |
| 900             | 3.832×10$^{-5}$               | 1.581×10$^{-11}$              | 2.427×10$^{-7}$                     | 0.696 | 2.515×10$^{-14}$ |
| 850             | 1.879×10$^{-6}$               | 8.452×10$^{-6}$               | -                                   | 0.998 | 1.042×10$^{-16}$ |
| 800             | 6.457×10$^{-7}$               | 9.149×10$^{-6}$               | -                                   | 0.980 | 3.662×10$^{-16}$ |
| 750             | 3.803×10$^{-7}$               | 1.067×10$^{-5}$               | -                                   | 0.990 | 1.023×10$^{-16}$ |
| 700             | 2.526×10$^{-7}$               | 1.888×10$^{-10}$              | -                                   | 0.875 | 8.707×10$^{-16}$ |

Figure 1. Linearisation of oxygen permeation fluxes of SDC-SCFZ disc membrane between 700 and 950 °C. Symbols perform experimental results, whereas lines perform values calculated from (a) Zhu model (b) Xu-Thomson model.

3.3. Distribution of resistances

The distribution of permeation resistances is determined as a product of temperature between 700 and 950 °C at two distinct permeate side oxygen partial pressures, $P_{O_2}^{III}$ of 0.02 and 0.005 atm whereby the feed side oxygen partial pressure, $P_{O_2}^{I}$ is fixed at 0.21 atm (figure 2). At $P_{O_2}^{III}$ of 0.02 atm, an increase in $r''$ is observed between 700 and 850 °C. Such increase is compensated by the equal decrease in the distribution of resistance from $r'$. Above 850 °C, the distribution of resistance from surface exchange reaction reduces significantly whereas distribution of resistance from bulk diffusion, $r^b$ increases and accounts for approximately 95% of the total resistance at 900 °C. When $P_{O_2}^{III}$ is decreased to 0.005 atm, the distribution of resistance from $r''$ increases significantly relative to $P_{O_2}^{III}$ of 0.02 atm. The same trend in $P_{O_2}^{III}$ of 0.02 atm is observed when temperature rises above 850 °C and $r^b$ is involved. This indicates the limiting case changed from surface exchange reactions to mixture of surface exchange reactions and bulk diffusion at 850 °C. Furthermore, bulk diffusion becomes the main resistance contributor as compared to surface exchange reactions when temperature rises above 900 °C.
Figure 2. Distribution of permeation resistance between 700 and 950 °C at $P_{O_2}^f$ of 0.21 atm and $P_{O_2}^p$ of (a) 0.02 atm (b) 0.005 atm.

3.4 Activation energy

The activation energies, $E_a$ of fluxes calculated based on $r'$ and $r''$, $r^b$, and $r^{tot}$, are determined at feed side partial pressure of 0.21 atm and permeate side partial pressure of 0.02 atm (figure 3). Two different $E_a$ for both limiting cases and $r^{tot}$ are observed, which indicate the change in the limiting case at 850 °C. An $E_a$ of 117.8 ± 12.8 kJ mol$^{-1}$ was attained for the flux based on $r^{tot}$ at high temperature region (850–950 °C). In this region, the activation energies for fluxes based on surface exchange resistances and bulk diffusion resistances are similar, which suggests that the oxygen transport is limited by a mixture of surface exchange reactions and bulk diffusion. At low temperature region (700–850 °C), an $E_a$ of 71.9 ± 13.4 kJ mol$^{-1}$ was attained for the fluxes based on $r^{tot}$, which is comparable to the $E_a$ calculated from the regression of fluxes based on surface exchange resistances (69.4 ± 13.4 kJ mol$^{-1}$). This tallies with the earlier assumption that the fluxes are limited by surface exchange reactions between 700 and 850 °C.

Figure 3. Arrhenius plot of the oxygen permeation fluxes determined based on $r'$ and $r''$, $r^b$, and $r^{tot}$ under oxygen partial pressure gradient of 0.21/0.02 atm (feed/permeate).
3.5. Influence of oxygen partial pressure variation

Figure 4(a) illustrates the oxygen permeation fluxes as a product of feed side pressure, \( P_{\text{air}} \) at 850 and 950 °C, at two distinct permeate side oxygen partial pressures, \( P_{O_2}^{II} \) of 0.1 and 0.02 atm. At each individual temperature and permeate side oxygen partial pressure, the increase in \( P_{\text{air}} \) brings about an increase of oxygen permeation flux. At \( P_{O_2}^{II} \) of 0.1 atm, the oxygen permeation fluxes at 850 °C is higher than at 950 °C above the crossover point, \( P_{\text{air}} \) of 12 atm. This may be attributed to the additional denominator term \((k_1 0.5k_2 0.5P_{O_2}^{II} 0.5P_{O_2}^{III} 0.5}) \) in equation 5 that may contribute to lower oxygen permeation fluxes at 950 °C as compared to 850 °C with increasing \( P_{\text{air}} \) and \( P_{O_2}^{III} \) of 0.1 atm. At \( P_{O_2}^{III} \) of 0.02 atm, the additional term in the denominator of equation 5 is smaller in value, and the flux is not reduced as much as that at \( P_{O_2}^{II} \) of 0.1 atm.

![Figure 4(a)](image1)

**Figure 4.** Influence of variation in \( P_{\text{air}} \) at 850 and 950 °C.

Figure 4(b) illustrates the oxygen permeation fluxes as a product of \( P_{O_2}^{II} \) at 850 and 950 °C, and at two distinct \( P_{\text{air}} \) of 1 and 5 atm. A decrease in \( P_{O_2}^{II} \) brings about an increasing trend in oxygen permeation flux at 950 °C and a decreasing trend at 850 °C. This is attributed to the increase in \( r^{''} \) at 850 °C along with the decrease in \( P_{O_2}^{II} \) (figure 4), which brings about a decrease in oxygen permeation flux. In contrast, the \( r^{''} \) at 950 °C remains unchanged and thus leads to an increase in flux. Increasing the feed side pressure from 1 to 5 atm is expected to boost the oxygen permeation fluxes by an average of 5.65×10⁻⁷ and 5.14×10⁻⁷ mol s⁻¹ cm⁻² at 850 and 950 °C, respectively. However, the increase of oxygen permeation fluxes from 1 to 5 atm at 950 °C is found to be more stable than at 850 °C. Therefore, operating the membrane at higher temperature will exhibit more stable and higher oxygen permeation flux.

![Figure 4(b)](image2)

**Figure 4.** Influence of variation in \( P_{\text{air}} \) at 850 and 950 °C.

4. Conclusion

In conclusion, the Zhu model is more applicable for the simulation of oxygen permeation fluxes of dual-phase SDC-SCFZ disc membrane as compared to the Xu-Thomson model given the overall good correlation and low sum of squared error. The oxygen transport is found to be limited by surface exchange reactions between 700 and 850 °C and a mixture of surface exchange reactions and bulk diffusion above 850 up to 950 °C. Bulk diffusion is revealed as the main resistance contributor above 900 °C. Through a parametric study, the increase in feed side pressure, \( P_{\text{air}} \) from 1 to 30 atm increases the oxygen permeation flux. Decreasing the permeate side oxygen partial pressure, \( P_{O_2}^{II} \) from 0.1 to 0.01 atm
increases the oxygen permeation flux for 950 °C but decreases for 850 °C. As such, SDC-SCFZ disc membranes exhibit high oxygen flux up to \(2 \times 10^{-6} \text{ mole s}^{-1} \text{ cm}^{-2}\) at 950 °C with \(P_{\text{air}}\) of 5 atm but \(P_{\text{O}_2}\) of 0.005 atm. Thus, SDC-SCDZ disc membrane indicates higher oxygen flux than other dual-phase membranes mixed with ionic and electronic conductor. The optimum range of operating conditions to maximise the oxygen permeation flux for SDC-SCFZ disc membrane are at 950 °C with \(P_{\text{air}}\) of 1 atm and \(P_{\text{O}_2}\) lower than 0.025 atm. This work is significant in providing insights of SDC-SCFZ disc membrane and further improvement of similar membrane compositions can be developed based on optimum operating conditions found in this work. To further extend this work, it is recommended to conduct the simulation using different membrane compositions to determine the extent of the applicability of the Zhu model.

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