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Numerical investigation of a hybrid polymeric-ceramic membrane unit for carbon-free oxy-combustion applications

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ABSTRACT

This work aims at developing a hybrid polymeric/ceramic membrane unit for oxy-fuel combustion applications. A ceramic oxygen transport membrane (OTM) unit is integrated numerically with a polymeric membrane unit to form the hybrid polymeric-ceramic membrane reactor. Oxygen-enriched air out of the polymeric membrane unit is fed to a ceramic membrane oxy-fuel based reactor. A detailed numerical study is performed to investigate oxy-fuel combustion in a tubular oxygen transport reactor (OTR) that is fed by oxygen-enriched air. CH_4/CO_2 mixture with various concentrations is swept inside the tubular OTR, where CO_2 serves as a diluent. The effects of sweep gas flow rate, feed gas flow rate, fed O_2 mass fraction, and swept CH_4 mass fraction on permeation fluxes and combustion process are investigated. Energy and design analyses of the hybrid membrane unit are conducted and the ratio between the required fiber polymeric membranes area to the ceramic membranes area is calculated as a function of the sweep flow rate. It was found that stoichiometric combustion within the OTR is achievable at a certain feed flow rate. The output power of the hybrid membrane unit is calculated and compared with the output power in case of air fed unit (without the polymeric membranes).

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1. Introduction

Oxy-fuel combustion is considered to be one of the most promising carbon capture technologies toward the control of global warming issue. Pure oxygen or oxygen-enriched air could be generated by three main air separation methods including; cryogenic distillation, pressure swing adsorption, and membrane separation. Cryogenic distillation is the most common of these three technologies and produces oxygen of more than 99% purity with large scale production [1]. Pressure swing adsorption can reach up to 95% oxygen purity, but the requirement of solvents limits its size capacity. This is primarily due to capital costs [2,3]. The membrane separation technology is the most recent of these three technologies. This technology utilizes high temperature ceramic ion transport membranes (ITMs) and polymeric membranes. Polymeric membranes for gas separation have been studied extensively in the literature targeting the development of high performance membranes for different applications [4–6]. One of the recently developed groups of membranes is the thermally rearranged (TR) polymeric membranes group by Park et al. [4]. These polymeric membranes have high selectivity and high permeability for different gases. Various studies were conducted to develop polymers from this family and to explore the gas separation process through this type of membranes [5–8]. Dong et al. [9] solved a model for gas separation in a TR-PBO hollow fiber membrane using MATLAB, and they proposed to include the shell-side pressure drop while modeling gas separation. Choi et al. [10] performed a study on O_2 removal from exhaust gas streams using polymeric membrane for complete capture of CO_2. They evaluated the permanent changes in polymer morphology and separation performance data considering single gas permeation.

The use of ceramic ion transport membranes (ITMs) allows production of highly pure oxygen through air separation at high temperature (more than 973 K) and high pressure and at reduced costs [11]. ITMs have high oxygen selectivity compared to polymeric membranes, but they only operate at high temperatures that could eliminate their utility for high temperature applications [12].

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However, ITMs can be a good choice for oxy-fuel combustion applications, as the combustion process provides the required heat to raise the membrane temperature for air separation [13]. Increasing O2 concentration on the feed side through using oxygen-enriched air instead of atmospheric air enhances the partial pressure difference across the membrane resulting in higher oxygen permeation rate. This oxygen-enriched air stream can be generated through the use of polymeric membranes. In this case, atmospheric air is fed to the polymeric membrane in the feed side to produce oxygen-enriched air mixture in the permeate side, which can be fed to the ceramic membrane unit [14]. Polymeric membranes can produce oxygen-enriched air with more than 50% mole fraction, depending on the polymer type. The present research study aims at developing a hybrid polymeric-ceramic membrane unit for oxy-fuel combustion applications. In these hybrid membranes, the oxygen-enriched air out of the polymeric membrane unit is fed to an oxygen transport reactor (OTR) unit for oxygen separation and oxy-combustion of gaseous fuel.

The performance of different types of ceramic membranes for pure oxygen separation has been investigated extensively in the literature with little emphasis on oxygen permeation under oxy-combustion conditions [13–17]. Yantovski et al. [15] used ITM to feed oxygen for an oxy-fuel combustion power plant. They found that the corresponding turbine inlet temperatures ranged between 1573 K and 1773 K and the thermal efficiencies ranged from 46 to 55%. Habib et al. [13] modeled an isothermal multi-channel reactor for oxy-fuel combustion to study the permeation and combustion behavior at different operation conditions. It was found that the reactions in the permeate side lead to an increase in the oxygen partial pressure gradient across the membrane as well as the membrane temperature, thereby, oxygen permeation flux increased. Nemitallah et al. [16] initiated a numerical study to investigate the performance of an ITM reactor under oxy-combustion conditions and the effect of various parameters on the reactor operation. Hong et al. [17] numerically investigated laminar oxy-fuel diffusion flames in the permeate side of an ITM. They found that the flame location affects the heat transfer and species diffusion from the reaction zone to the ITM, which affects the flame temperature and the oxygen permeation flux.

Cryogenic distillation, the most conventional method of air separation, is an expensive method and does reduce the plant's efficiency [18]. Burdyny and Struchtrup [19] studied the air separation using a hybrid membrane-cryogenic system for small and medium oxy-fuel systems. The results showed that the process efficiency could be improved by 0.9% in this hybrid system. In the present study, Fluent software is utilized to perform a detailed numerical study on the characteristics of air separation and oxy-fuel combustion in a hybrid polymeric-ceramic membrane unit. The produced oxygen-enriched air from the polymeric membrane is fed to the ceramic oxygen transport reactor (OTR) to build the hybrid system. User defined functions (UDFs) written in visual C++ are coupled and hooked to the Fluent software to account for the transfer of both oxygen and nitrogen across the polymeric membrane and the transfer of oxygen only across the ceramic membrane. Effects of different parameters on the permeation characteristics and the oxy-fuel combustion process in the OTR are investigated. A proposed design of the hybrid unit is presented in the present work.

2. Model development and solution methodology

2.1. Modeling of polymeric membrane unit

Recently, we have carried out a detailed numerical study trying to understand the characteristics of air separation in hollow-fiber polymeric membrane unit targeting the production of oxygen-enriched air for clean combustion applications [20]. In this study, a shell and tube design of a polymeric membrane unit is considered, and 2-D numerical simulations were performed considering asymmetric single hollow fiber membrane unit with its surrounding shell. The same polymeric membrane unit is used in the present study with the same configuration as in Ref. [20], and the simulation results are utilized in the present study for the development of a hybrid polymeric-ceramic membrane unit for oxy-combustion applications. Oxygen-enriched air stream leaving the polymeric membrane unit is utilized as feed flow for the oxygen transport reactor (OTR) ceramic membrane unit. Counter-current flow bore-side feed configuration was considered in this model to give better separation results [21]. Air (20.5% O_2 and 79.5% N_2, by volume) is fed to the fiber membrane cell in the bore-side, and oxygen depleted air leaves as retentate at the end of the feed side. While at the shell-side, oxygen-enriched air is produced. This is utilized to feed the oxygen transport reactor (OTR) in the hybrid system. Pressure outlet conditions have been specified at the permeate and feed outlets (atmospheric pressure at the permeate outlet and 10.13 bar at the feed outlet). Mass flow rate inlets boundary conditions have been assigned for the sweep and the feed entries.

The numerical model of the polymeric membrane gas separation unit was established and validated using Fluent software. The numerical solution of the flow field includes the solution of the partial differential equations of continuity, energy, momentum, and species transport. The equations are presented as follows [22]:

$$\nabla\cdot(\rho U) = S_i \tag{1}$$

$$\nabla\cdot(\rho UU) = -\nabla p + \mu\nabla^2 U \tag{2}$$

$$(\rho C_p)_f U\cdot\nabla T = \nabla\cdot\left(k_f\nabla T\right) \tag{3}$$

$$\nabla\cdot(\rho U X_i) - \nabla\cdot\left(\rho D_{i,m}\nabla X_i\right) = S_i \tag{4}$$

Where U is the velocity, μ is the dynamic viscosity, ρ is the density, p is the pressure, $D_{i,m}$ is the diffusion coefficient in the mixture, T is the temperature, and X_i is the mass fraction. Source/sink term, S_i, was used to consider the transfer of O_2 and N_2 across the polymer membrane. To include this source/sink term in the governing equations as presented above, user defined functions (UDFs) were written in Visual C++ and compiled and hooked to the Fluent software to close the set of the governing equations [22]. The law that controls the fluid flow through a porous medium, which was used to solve for the permeation across the polymer membrane, can be expressed as follows [23]:

$$J_{O_2/N_2} = \frac{P(p' - p'')}{L} \tag{5}$$

Where J is the permeation flux of O_2 or N_2 in mol/m^2/s and P is the permeability of the polymer membrane in mol.m/m^2/s/Pa. p' and p'' are the gas partial pressure in the feed and the permeate sides, and L is the membrane thickness. Based on the flux equation, the equation of the source/sink term is developed for both O_2 and N_2 at each boundary membrane cell. A grid independence study has been performed to select the appropriate mesh size and to make sure that the results are independent of the mesh size [20]. Experimental data by Feng et al. [21] were used to validate the present model for polymeric membrane system. More details about the polymeric model and its validation are illustrated in detail in our previous work [20].

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