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Numerical study of gas separation using a membrane

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ABSTRACT

Computational fluid dynamics simulations are conducted for multicomponent fluid flows in a channel containing spacers. A new and unique model has been presented for the treatment of the membrane boundaries in the separation CO_2 from CH_4 in a binary mixture. The equation governing the flux through the membrane is derived from first principles. The membrane is modeled as a functional surface, where the mass fluxes of each species will be determined based on the local partial pressures, the permeability, and the selectivity of the membrane. The approach introduced here is essential for simulating gas–gas separation. Baseline Reynolds stress, k–ω BSL, and large eddy simulation, LES, turbulence models are employed to study spatial and temporal characteristics of the flow for Reynolds number up to 1000. It is shown here that the spacers have a strong effect on the membrane performance. The process of separating CO_2 from CH_4 is improved by the presence of spacers in the membrane system. It is demonstrated that spacers should be an integral part of the membrane system design in the application of gas–gas separation.

1. Introduction

Natural gas consumption has increased significantly in recent years. The impurities found in raw natural gas, extracted from underground, should be minimized to protect pipelines from corrosion. Membranes are used to separate these undesired gasses, thereby purifying the natural gas. In order to minimize capital and operation costs of the purification process, the membrane performance needs to be enhanced.

In this study, flows of a binary mixture, CH_4 and CO_2, in a channel bounded by two membranes are studied for a wide range of Reynolds numbers. Cases, with and without spacers of varying sizes and shapes, are considered. The steady flow, bounded by the membrane walls, is characterized by a simple laminar flow model in the case without any spacers, and by a k–ω baseline Reynolds stress turbulent model in the case with spacers. A unique model is presented for the treatment of the membrane boundaries; with which CO_2 absorption and CH_4 losses through the membrane are calculated for both cases. The membrane flux model, derived from basic principles by the present authors, is necessary to accurately represents gas separation and is valid for the desalination process in the limit the concentration of the one of the component tends to zero.

In the past, gas–gas separation using a membrane had been studied extensively by several investigators. Such studies include: improving the permeability and the selectivity of the membrane [1–5]; operating the membrane at the optimum temperature and pressure [6–8]; or improving the separation modules [9–11]. In this study, the focus is less on these aspects of separation and more on enhancing the membrane performance using momentum mixing. This is a well-known and studied alternative approach for improving membrane performance. There have been extensive studies which show that enhanced momentum mixing in an open channel improves membrane performance in water treatment. However, the effect of mixing on the membrane's performance in gas–gas separation has not been studied.

Several investigations study the effects of momentum mixing on the membrane performance without considering the mass transport. Karode and Kumar [12] and Saeed et al. [13] consider a steady 3D laminar flow model to study the effects of a cylindrical spacer on the pressure drop at low Reynolds number. Fimbres-Weihs et al. [14] and Ranade and Kumar [15] employed a direct numerical simulation (DNS) of the Navier–Stokes equation to study the effects of a cylindrical spacer on the pressure drop and the drag coefficient for a wide range of Reynolds numbers reaching above 1000. They have reported that the critical Reynolds number for the onset of transition from steady to unsteady flow occurs at around 300. Schwinge et al. [16] have studied how the staggered and the inline cylindrical spacers affect the flow field using direct

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Nomenclature

A	surface area [m]
D	diffusion coefficient [m^2/s]
L	channel length [m]
$\bar{P}$	permeability $\left[\frac{mole}{m\ s\ pa}\right]$
Re	Reynolds number [–]
Sc	Schmidt number [–]
S	spacing between spacers [m]
U	average velocity [m/s]
Y	mass fraction [–]
h	channel height [m]
k	turbulent kinetic energy [J/kg]
m	mass flux [$kg/m^2/s$]
Δp	pressure difference [Pa]
τ	stress tensor
v	y-component of the velocity [m/s]
y	y coordinate [m]
$\bar{\alpha}$	molar selectivity [–]
ρ	density [kg/m^3]
β^*, β_1, β	turbulent model parameters [–]
C	concentration [$mole/m^3$]
J	molar flux [$mole/m^2$]
M	molecular weight [g/mole]
P	permeance $\left[\frac{g}{m^2\ s\ Pa}\right]$
Sh	Sherwood number [–]
F_1	blending function [–]
St	staggered offset [m]
V	suction rate [m/s]
d	spacer diameter [m]
h_m	mass transfer coefficient [m/s]
l	membrane thickness [m]
p	pressure [Pa]
u	x-component of the velocity [m/s]
γ	rate of strain tensor
x	x coordinate [m]
υ	kinematic viscosity [m^2/s]
α	mass selectivity [–]
ω	specific dissipation rate [1/s]
σ, λ	turbulent model parameters [–]

Subscripts

a and b	species: CO_2 or CH_4
i and j	index notation
CH_4	properties of CH_4
tot	total properties
T	eddy properties
CO_2	properties of CO_2
w	properties at the membrane

numerical simulations. Ranade and Kumar [17] considered a 3D k–ε turbulent model to study the effects of cylindrical spacers on the pressure drop at Reynolds numbers above 350. In the present study, so as to model the effects of the membrane, a mass transport equation is introduced and the membrane is modeled as a functional surface through which the mass flux is determined by the local pressures and the local concentration. Several studies also introduced a mass transport equation, but still treated the membrane as an impermeable wall. Al-Sharief et al. [18] and Shakaib et al. [19] consider a 3D laminar Navier–Stokes model to study the effects of cylindrical spacers on the mass transfer in a water desalination process. A mass transport equation was also introduced by Al-Sharief et al. [18] assumed the mass flux of salt is constant on the membrane; an assumption which can be safely made in desalination studies, but not in gas–gas separation. Shakaib et al. [19] assumed constant concentration on the membrane. Several investigations improved upon the idea of treating the membrane as a permeable wall. Pal et al. [20] studied the effect of cylindrical spacers on membrane performance in the food industry. The membrane flux was assumed to be constant and a constant concentration on the membrane was assumed on a 2D laminar flow model. Subramani et al. [21] and Guillen and Hoek [22] assumed that the flux through the membrane was constant and that the mass flux of the solute was constant. Both of them used a 2D laminar flow model to simulate the flow behavior in water treatment. Subramani et al. [21] studied two parallel membranes without spacers. Guillen and Hoek [22] studied the effects of different shapes of spacers on the membrane performance. Not considered in these previously mentioned studies, real separation processes need to consider the flux through the membrane as a function of the local pressure and osmosis pressure. Lyster and Cohen [23], Villaluenga and Cohen [24] and Fletchera and Wiley [25] considered the local pressure and osmosis pressure in their models. They assumed the mass flux of the salt was linearly proportional to that of the water. All of these studies considered a flow with two parallel membranes without any spacers. With a similar membrane treatment as what was seen in these aforementioned papers [23–25], Fimbres-Weihs and Wiley [26] used a 3D laminar model to study the effects of spacer orientation on the membrane performance. Ahmad and Lau [27], Lau et al. [28], Ma and Song [29] and Ma et al. [30] used DNS to solve the Navier–Stokes equation for flow between two membranes with spacers. Ahmed and Lau studied the effects of different shapes of spacer attached on the membrane and Lau et al. [28] studied the effects of cylindrical spacers on membrane performance. Ma and Song [29] and Ma et al. [30] studied the effects of varying placements of square spacer on the membrane performance.

The aforementioned studies were focused on water desalination with membranes. The concentration of the salt in saline water ($mole_{salt}/mole_{water}$) varies from 0.002 to 0.04. The salt flux on the membrane is negligible when compared with the water flux. For the mass transport through the membrane, the salt flux can be assumed to be linearly proportional to the water flux. However, neither assumption can be used in the gas–gas separation where the concentrations of both species are comparable. In a model for gas–gas separation, the flux of both species has to be considered in the momentum and mass transports through the membrane. In the present study, the model presented considers these effects. This makes the model presented unique in both its ability to accurately model gas–gas separation flows and in its adaptability to other membrane flow applications. There exists no previous model which could study these flows without making some of the aforementioned assumptions about the membrane.

2. Governing equations

Steady two dimensional flows of CH_4 and CO_2 binary mixture in a channel bounded by two parallel membranes are studied here for Reynolds number from 200 to 1000 using a k–ω baseline Reynolds stress turbulence model. Transient two dimensional simulations are also conducted using both large eddy simulations (LES) and a k–ω BSL turbulence model for $Re = 800$ to investigate the effect of vortex shedding on the mass transport through the membrane.