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Optimization of hollow fiber membrane modules to sequester carbon dioxide from coalbed methane

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ABSTRACT

A novel optimization method, based on a mathematical modeling approach, for the design and operation of a hollow fiber membrane module is developed. The purpose of the membrane is to purify unconventional gases, such as coalbed methane gas, by removing carbon dioxide. For the design of the membrane module, the number of fibers within the module must be reasonably set as one of the design variables of the optimization problem. Therefore, a mixed integer nonlinear programming (MINLP) model including integer variables – i.e., the number of fibers in this study – is required to obtain optimal design conditions. However, if the integer variable is involved in the highly nonlinear model, the probability of success in the optimization calculation becomes very low because of the big computation load. Thus, this paper introduces: (1) a new optimization modeling technique which is able to solve the MINLP problem efficiently; (2) a successful scale up design optimization from laboratory (0.5 Nm^3/h) to large commercial scale (500 Nm^3/h); (3) design optimization results under different gas feed conditions, and (4) dynamic optimization results obtained by varying gas feed conditions.

1. Introduction

Membranes have become a promising technology in the area of gas separation due to their compactness, energy savings, reduced capital investment cost, simple operation, easy offshore installation, and the convenient integration with any other separation system. For designing the membrane, mathematical modeling and simulation are very useful tools as they can reduce the number of experiments, the time, and the costs of the designing process. In addition to the system's simulation, optimization techniques can be used to find more efficient designs for the membranes.

A number of papers have been published in the open literature focusing on the optimization of membrane-based gas separation systems. Several researchers performed the optimization studies considering the membrane configuration as one of the optimization targets. Qi and Henson (2000) performed a simultaneous optimization of a permeator configuration and its operating conditions using the mixed integer nonlinear programming (MINLP) design technique [1]. Lababidi et al. developed mathematical models to optimize three configurations for membrane gas separation modules including a single stage, two stages, and the continuous membrane column [2]. Datta and Sen focused on finding the optimum configuration and design variables for the asymmetric membrane-based separation of carbon dioxide from natural gas for satisfying the pipeline specification of 2% of carbon dioxide [3]. Kookos introduced a new approach optimizing the membrane material together with the structure and the parameters of the membrane network [4]. Purnomo and Alpay designed and analyzed two generalized membrane configurations with recycle streams for the bulk air separation [5] by using the equation oriented gPROMS modeling software [6] with successive reduced quadratic programming (SRQP) optimization solver. Genetic algorithms were also employed for the membrane optimization by Marriot and Sørensen [7], and Chang and Hou [8]. Marriot and Sørensen reported an optimal design strategy for membrane separation systems based on genetic algorithms [7]. Chang and Hou applied genetic algorithm for the optimization of the membrane gas separation system with single and triple objective functions [8]. Tessendorf et al. introduced a mathematical model and a numerical solution procedure for the separation of multicomponents mixtures using a membrane gas module and implemented the simulation modules in the industrial equation oriented simulation and optimization environment, called OPTISIM developed by Linde AG [9].

Though a number of optimization studies have been carried out, there have been few works focusing on the optimization of the membrane module design based on a dynamic simulation model. The dynamic model can predict the dynamic behavior of the systems according to variations on the system's conditions within time and unexpected disturbances in real site situations. Thus, this paper focuses on the design optimization of the membrane module and the dynamic optimization of the system's operation. The adopted system is a hollow fiber membrane module with counter-current flow for CO_2 removal

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Nomenclature

A_{eff} effective membrane area (m^2)
$A_{I,\text{fiber}}$ fiber inside area (m^2)
$A_{\text{shell,void}}$ cross sectional shell void area (m^2)
$C_{\text{Pg,ave,fiber},j}$ average heat capacity of a bore side (J/K) in the discretized section j, $j = 1, \ldots, N_{dis}$
$C_{\text{Pg,ave,shell},j}$ average heat capacity of a shell side (J/K) in the discretized section j, $j = 1, \ldots, N_{dis}$
$D_{I,\text{fiber}}$ fiber inside diameter (m)
$D_{O,\text{fiber}}$ fiber outside diameter (m)
D_{shell} shell inside diameter (m)
$D_{\text{ave,fiber}}$ average of inside fiber diameter and outside fiber diameter used in this study instead of log mean diameter difference (m)
$D_{\text{hyd,shell}}$ hydraulic shell diameter (m)
$dV_{\text{shell,void}}$ discretized shell inside void volume (m^3)
dz discretized section length in an axial direction (m)
$dV_{I,\text{fiber}}$ discretized fiber inside volume (m^3)
$dA_{I,\text{fiber,wall}}$ discretized fiber inside wall area (m^2)
$h_{\text{fiber},j}$ enthalpy of a bore side (J/mole) in the discretized section j, $j = 1, \ldots, N_{dis}$
$h_{I,\text{fiber,wall}}$ heat transfer coefficient of an inside fiber wall (J/(m^2 s K))
$h_{\text{shell},j}$ enthalpy of a shell side (J/mole) in the discretized section j, $j = 1, \ldots, N_{dis}$
$h_{O,\text{fiber,wall}}$ heat transfer coefficient of an outside fiber wall (J/(m^2 s K))
L_{eff} effective length of a membrane module (m)
N_{dis} number of discretized sections
N_f number of fibers within a shell module
$n_{t,\text{fiber},j}$ overall mole number of bore side in the discretized section j (mole), $j = 1, \ldots, N_{dis}$
$n_{t,\text{shell},j}$ overall mole number of shell side in the discretized section j (mole), $j = 1, \ldots, N_{dis}$
$\dot{n}_{t,\text{shell},j}$ overall shell side molar flow rate (mole/s)
$\dot{n}_{t,\text{fiber},j}$ overall bore side molar flow rate (mole/s)
$P_{\text{fiber},j}$ pressure within a fiber in the discretized section j (Pa), $j = 1, \ldots, N_{dis}$
$P_{\text{shell},j}$ pressure within a shell in the discretized section j (Pa), $j = 1, \ldots, N_{dis}$
$Purity_{CH_4,\text{retentate}}$(%) methane purity
Q_i permeance of component i (mol/(m^2 s Pa))
$Recovery_{CH_4,retentate}$(%) methane recovery
$R_{t,j}$ overall permeation molar flow rate of total fibers in the discretized section j (mole/s), $j = 1, \ldots, N_{dis}$
$R_{i,\text{fiber},j}$ permeation molar flow rate of component i of each fiber (mole/s) in the discretized section j, $j = 1, \ldots, N_{dis}$
$StageCut$ stage cut
$T_{\text{shell},j}$ temperature within a shell in the discretized section j (K), $j = 1, \ldots, N_{dis}$
$T_{\text{fiber,wall},j}$ outside fiber wall temperature (K) in the discretized section j, $j = 1, \ldots, N_{dis}$
$T_{\text{fiber},j}$ temperature within a fiber in the discretized section j (K), $j = 1, \ldots, N_{dis}$
$u_{\text{shell},j}$ shell side gas velocity as to the axial direction (m/s) in the discretized section j, $j = 1, \ldots, N_{dis}$
$u_{\text{fiber},j}$ bore side gas velocity as to the axial direction (m/s) in the discretized section j, $j = 1, \ldots, N_{dis}$
$\dot{V}_{\text{feed},N}$ feed flow rate at normal condition (Nm^3/h)
$\dot{V}_{\text{permeate},N}$ permeate flow rate at normal condition (Nm^3/h)
$y_{\text{CH4,feed}}$ methane feed mole fraction
$y_{\text{CO2,feed}}$ carbon dioxide feed mole fraction
$y_{i,\text{fiber},j}$ mole fraction of component i within a bore side in the discretized section j, $j = 1, \ldots, N_{dis}$
$y_{i,\text{shell},j}$ mole fraction of component i within a shell side in the discretized section j, $j = 1, \ldots, N_{dis}$
$Z_{\text{fiber},j}$ compressibility factor of bore side in the discretized section j (mole), $j = 1, \ldots, N_{dis}$
$Z_{\text{shell},j}$ compressibility factor of shell side in the discretized section j (mole), $j = 1, \ldots, N_{dis}$

Greek letters

$\mu_{\text{fiber},j}$ viscosity of a bore side (kg/(m s)) in the discretized section j, $j = 1, \ldots, N_{dis}$
$\mu_{\text{shell},j}$ viscosity of a shell side (kg/(m s)) in the discretized section j, $j = 1, \ldots, N_{dis}$
$\rho_{g,\text{fiber},j}$ gas density of a bore side (kg/m^3) in the discretized section j, $j = 1, \ldots, N_{dis}$
$\rho_{g,\text{shell},j}$ gas density of a shell side (kg/m^3) in the discretized section j, $j = 1, \ldots, N_{dis}$

from coalbed methane (CBM) gas. Hollow fiber membrane modules have attracted a lot of interest in gas separation membranes due to their high productivity per volume unit, low production cost [10,11] and self-supporting characteristics [11].

This work introduces (1) the development of a new optimization modeling technique for membrane module design, and (2) the application of this technique to scale up designs, design optimizations, and dynamic optimizations based on the developed dynamic membrane model as shown in Table 1 [12].

This paper is organized as follows. First, the mathematical model and the new optimization modeling approach are explained in Section 2. In the next section, Section 3, the optimization results are presented. Section 4 is the last section and summarizes this study.

2. Mathematical formulation of hollow fiber membrane

The studied system is a hollow fiber membrane module that includes thousands of fibers inside the shell module. As can be seen in Fig. 1, the feed gas consisting of methane and carbon dioxide enters the bore side, and carbon dioxide permeates more through the fiber membrane walls than methane. Consequently, the carbon dioxide rich gas flows in the shell side as permeate streams and the purified methane gas is produced at the end of the retentate streams from the bore side. The adopted flow pattern is a counter-current configuration. The module in the axial direction is divided into N_{dis} compartments, and each compartment is assumed as continuous stirred tank reactor (CSTR).

The following assumptions are employed [12]:

- Hagen-Poiseuille equation used for pressure drop calculation.
- Negligible deformation of the fiber under the pressure.
- Uniform fiber radius
- Temperature-independent permeability.
- Adiabatic membrane module between outside wall of module and atmosphere.
- Negligible time derivative of pressure and compressibility factor.
- Redlich-Kwong-Soave equation of state.
- No radial variations of variables.

To determine the optimal design variables including discrete (integer) and continuous variables, the mixed integer nonlinear programming (MINLP) optimization problem needs to be solved. However, a MINLP problem is more difficult to be resolved by optimization solvers than a general nonlinear programming (NLP) problem. The hollow