Journal of Membrane Science 523 (2017) 77–91

Contents lists available at ScienceDirect

Journal of Membrane Science

journal homepage: www.elsevier.com/locate/memsci

Rigorous variable permeability modelling and process simulation for the design of polymeric membrane gas separation units: MEMSIC simulation tool

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ARTICLE INFO

Keywords:
Membrane
Separations
Permeability
Simulation
Design
Gas
Polymers

ABSTRACT

Membrane processes are, together with cryogeny, absorption and adsorption, a key technology for gas separation applications. For simulation purposes, a constant membrane permeability hypothesis is most often assumed for each gas compound, for sake of simplicity. In this study, the incidence of variable (i.e. pressure dependent) permeability of gases or vapors through dense polymeric membranes on module separation performances or design is investigated through a simulation study. A dedicated computer software (MEMSIC) including multicomponent mixtures computations and extendable to Process System Engineering (PSE) softwares through a CAPE OPEN tool is described. The modelling approach offers, for the first time, a rigorous computation of transmembrane fluxes based on different solution-diffusion models (dual mode, Flory Huggins, ENSIC) for a set of absolute upstream and downstream pressure. This strategy differs from a classical flux expression, based on the dependency of permeability either upon upstream pressure or transmembrane pressure, which has been proposed up to now but can generate computational errors. A series of simulation case studies through glassy and rubbery membranes is reported; it shows that the constant permeability hypothesis can lead in some cases to significant design errors (i.e. required membrane surface area for a given set of specifications). Furthermore, significant differences are observed compared to the classical variable permeability approach making use of the product of permeability with pressure difference. Tentative guidelines for the identification of the key characteristics of a given system which require a variable permeability behavior to be taken into account are finally proposed.

1. Introduction

Membrane processes appear as an attractive technology for the development of sustainable chemical process industries. Membrane separations indeed combine a series of key advantages: continuous operation without a regeneration step (simple process), no phase change (energy efficient process), compact units due to the large specific surface area of modules (intensified process), physical separation process without chemical reactions involved and without wasted chemicals losses (environmental friendly process). For gas separation applications, membrane separations is nowadays considered as one of the key technologies, together with cryogeny, gas-liquid absorption and adsorption. In terms of materials, almost exclusively dense thin skin polymeric membranes are applied at industrial scale. Air separation, hydrogen purification, natural gas treatment, Volatile Organic Compounds recovery from air and gas drying operations are the major current markets of membrane gas separations [1]. Promising gas or vapor applications are expected to emerge such as post-combustion carbon capture, organic vapor separation for chemicals production (hydrocarbons, organic biomolecules) or renewable energy purification operations (biogas, hydrogen from electrolysis...).

In order to evaluate the potentialities of membrane gas separation processes for a target application, efficient modelling simulation approaches are obviously of major importance. A large number of publications have addressed the various process modelling possibilities for a steady state membrane gas separation unit, covering different levels of complexity. Basically, a great number of process studies make use of the reference case proposed by Weller and Steiner in their pioneering work [2]. This baseline approach is based on the following set of assumptions:

1. Steady state operation (no time dependency of fluxes)
2. Binary feed mixture
3. Isothermal conditions

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http://dx.doi.org/10.1016/j.memsci.2016.09.011
Received 22 July 2016; Received in revised form 8 September 2016; Accepted 10 September 2016
Available online 01 October 2016
0376-7388/