Data supporting the validation of a simulation model for multi-component gas separation in polymeric membranes

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ARTICLE INFO

Article history:
Received 28 September 2016
Received in revised form
19 October 2016
Accepted 21 October 2016
Available online 26 October 2016

Keywords:
Post-combustion CO₂ capture
Membrane separation
Model validation
Separation performances

ABSTRACT

The article describes data concerning the separation performances of polymeric hollow-fiber membranes. The data were obtained using a model for simulating gas separation, described in the research article entitled “Interplay of inlet temperature and humidity on energy penalty for CO₂ post-combustion capture: rigorous analysis and simulation of a single stage gas permeation process” (L. Giordano, D. Roizard, R. Bounaceur, E. Favre, 2016) [1]. The data were used to validate the model by comparison with literature results. Considering a membrane system based on feed compression only, data from the model proposed and that from literature were compared with respect to the molar composition of permeate stream, the membrane area and specific energy requirement, varying the feed pressure and the CO₂ separation degree.

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Specifications Table

| Subject area                  | Process engineering                  |
|-------------------------------|--------------------------------------|
| More specific subject area    | Post-combustion CO₂ capture          |

DOI of original article: http://dx.doi.org/10.1016/j.energy.2016.09.129
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http://dx.doi.org/10.1016/j.dib.2016.10.019
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The data describe the separation performances and the specific energy requirement of a single-stage membrane unit; hence they can be used in future works to compare simulation results of different membrane system models.

- The data contain key information regarding the performances of a single-stage membrane system operating the CO₂ capture from exhaust flue gases; hence these data can be used to support the study of more complex membrane separation systems, such as those based on dual-stage configuration.
- The data can be used by other researchers for a preliminary assessment of energy penalty inflicted to power plants integrating a post-combustion CO₂ capture system based on a single-stage membrane configuration.
- The data are valuable for other studies concerning the conceptual design of single-stage membrane systems for CO₂ capture reuse applications.

1. Data

Data shared in this article concern the validation of a model for evaluating the performances of a post-combustion CO₂ capture membrane system. Data consist of molar fractions of permeate stream, membrane area and specific energy requirement of membrane system. Data were obtained by varying the CO₂ separation degree from 0 to 100% and the feed pressure from 4 bar to 10 bar.

2. Experimental design, materials and methods

With the aim to validate a model for simulating the gas separation in polymeric hollow-fiber membrane modules [1], the related simulation data were compared with those obtained in a previous published paper by Low et al. [2], based on the same membrane system layout and operating conditions. Specifically, a single-stage configuration with feed compression only was simulated (Fig. 1). Gas separation in the membrane module was mimicked using the proprietary simulation tool M3PRO [3]; the latter was integrated in Aspen Plus environment [4], with the aim to simulate the energy behavior of the whole membrane separation system.

Table 1 summarizes the simulation operating conditions, including the membrane separation properties and the thermodynamic conditions of flue gas to be treated.

Fig. 2 compares the permeate composition evaluated with the model proposed (Fig. 2a and c) and that obtained by Low et al. [2] (Fig. 2b and d), varying the CO₂ separation degree and the feed pressure. It is noted that the trend of simulated data varying the CO₂ separation degree fits very well with the literature data. For instance, setting a feed pressure of 10 bar and increasing the CO₂ separation degree from 20% to 100%, Fig. 2a shows that in the proposed model CO₂ molar fraction reduces from around 70% to 30% and N₂ molar fraction increases from around 20% to 60%. Almost the
same values are observed in Fig. 2b, depicting the trend of permeate molar fractions evaluated in [2] with the same operating conditions. Additionally, both models show that CO₂ and N₂ molar fractions attain the same values (≈ 45%) for a CO₂ separation degree of around 90%. The good agreement is also confirmed at a lower feed pressure (4 bar), where both models show that CO₂ and N₂ molar fractions pass from 50% to 25% and from 40% to less than 70% respectively, for a corresponding increase of CO₂ separation degree up to 95% (Fig. 2c and d).

Fig. 3 compares the membrane area evaluated with the model proposed, for a feed pressure of 8 bar (Fig. 3a) and that obtained by Low et al. [2] (Fig. 3b) at the same operating conditions. The trend of membrane area evaluated with the proposed model fit well with that obtained in [2]. In this regards, it is noted that for both models membrane area has an exponential increase, stating at around 20 m² for a CO₂ separation degree up to 95% (Fig. 2c and d).

Table 1
Operating conditions for simulating the single stage membrane system with feed side compression.

| Parameter | Value |
|-----------|-------|
| x_CO₂, % mol | 14.7 |
| x_N₂, % mol | 76.2 |
| x_H₂O, % mol | 4.3 |
| x_O₂, % mol | 4 |
| x_Ar, % mol | 0.8 |
| m_EXH, Nm³/h | 100 |
| T_EXH, °C | 30 |
| p_EXH, bar | 1 |
| p_CO₂, Barrer | 150 |
| p_N₂, Barrer | 4.2 |
| p_H₂O, Barrer | 1500 |
| p_O₂, Barrer | 11.7 |
| p_Ar, Barrer | 11.7 |

Fig. 1. Layout of a single stage membrane system with feed compression only in Aspen Plus V8.4.
Fig. 2. Comparison between the permeate molar composition evaluated with the model proposed (a and c) and that from Low et al. [2] (b and d).

Fig. 3. Comparison between membrane area evaluated with the model proposed (a) and that from Low et al. [2] (b) for a feed pressure of 8 bar.
energy states at less than 250 kWh/tonne in [2], while it reduces to around 200 kWh/tonne in the proposed membrane system.

Acknowledgements

The study received the financial support from European Union’s Seventh Framework Program (FP7/2007-2013) under Grant agreement no. 608490, project M4CO2.

Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.10.019.

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