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

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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 CO ₂ capture

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Type of data	Table and Figures
How data was acquired	Numerical simulation
Data format	Raw
Experimental factors	No pretreatment of data was performed
Experimental features	The simulation of single stage membrane system was performed using a proprietary software tool integrated in Aspen Plus environment
Data source location	Nancy, France
Data accessibility	Data are provided within this article

Value of the data

- 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.
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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

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