Production of oxygen-enriched air via desorption from water: Experimental data, simulations and economic assessment

Federico Galli [a], Alberto Comazzi [a], Daniele Previtali [a], Flavio Manenti [b], Giulia Bozzano [b], Claudia L. Bianchi [a], Carlo Pirola [a],*

[a] Università degli Studi di Milano, Dipartimento di Chimica, Via Golgi 19, 20133, Milano, Italy
[b] Politecnico di Milano, Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", piazza Leonardo da Vinci 32, 20133, Milano, Italy

ABSTRACT

Oxygen enriched air with a composition of oxygen till 35% can be produced by water desorption by simple water degassing. This work reports the simulation of a small bench-scale plant for the continuous production of oxygen-enriched air by simple water degassing. The basic thermodynamic principle involved is the higher water solubility of oxygen compared to the one of nitrogen. Different experiments were performed in a continuous small bench-scale plant changing the main operating parameters, i.e. water temperature, degasser pressure and the water flowrate in order to develop rigorous and reliable simulations with suitable software (PRO/II 9.3 by SIMSCI-Schneider Electric). The results obtained showed a good fitting between the experiments and the simulations and demonstrated the possibility for the production of enriched air using this new technology. Moreover, the calculation of the economic potentials of this new process were carried out, and the results compared to the already existing technologies.

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1. Introduction

Among all the industrial processes that involve an oxidation step, air is the cheapest and most used oxidizing agent (Franz, 2005). Together with oxygen, atmospheric air also contains other gases, mainly nitrogen, which are inert and do not participate to the oxidation reaction. The presence of these inert compounds make compulsory the installation of bigger equipments to achieve the same conversion obtained by using pure oxygen. Oxygen enriched air (EA) consists of air in which the oxygen concentration is someway increased from the atmospheric value, i.e. 20.95% (Seinfeld and Wiley, 2006) up to about 35%. Its use in any process could significantly reduce the plant costs (Roadmap, 1999), both capital and operating (Gollan and Kieper, 1984), because smaller reactors can be used in order to obtain the same reactant conversion, using a lower amount of EA. This mixture can be potentially used to improve the efficiency of gas-liquids oxidations and in several chemical plants involving for example the Claus process, the Fluid Catalytic Cracking technology during the catalyst regeneration step, or in burners and wastewater treatment plants. Moreover, in particular cases like, for example, the oxidation of *p*-xylene to give

terephthalic acid, the introduction of EA increases the reaction yield (Cao et al., 1999).

Currently, different processes exist for the production of enriched air and the main two technologies rely on the air cryogenic separation (Belaissaoui et al., 2014) and the membrane separation (Bernardo et al., 2009). In both these technologies, the energy demand for the production of oxygen enriched air is intensive, thus different studies were elaborated for finding alternatives or solutions for the intensification of the process (Co, 2016). Recently, two of the authors of this work published a paper concerning a new process for the obtainment of oxygen enriched air together with a detailed analysis of the potential advantages by producing and employing in situ EA in a seawater desalination plant located in Pantelleria island (Italy) (Manenti and Pirola, 2014a). Oxygen enriched air was obtained by desorption from water, taking advantage of the higher oxygen solubility in water compared to the nitrogen one (Manenti and Pirola, 2014b), since the Henry constants of this two gases are different (Wilhelm et al., 1976). The main advantage of this new technology is that it can be coupled to any existing plant in which a stream of water is either someway heated or is obtained after a heat recovery from a steam stream. This kind of stream can be used for heating the water in the degassing unit for the production of EA. Since these streams represent a challenge for the heat recovery due their low heat flow (Papoulias and

* Corresponding author.
  E-mail address: carlo.pirola@unimi.it (C. Pirola).

Grossmann, 1983), this technology can make this kind of energy flow valuable.

The aim of the present paper is to show the feasibility of the EA production by desorption from water in a continuous lab-scale plant. The main operating parameters were varied (water flowrate, pressure and temperature of the degassing unit) in order to correlate them with the volume and oxygen concentration of the EA produced. Together with the experiments, static simulations using the software PRO/II 9.3 by SimSci-Schneider Electric were performed for checking the consistency of the results. Moreover, an economical assessment of this new technology was carried out calculating the main operating (OPEX) and capital (CAPEX) expenses using the Guthrie method (Guthrie, 1969; Guthrie, 1974). The cost of the EA produced was compared to the market price of the enriched air produced by typical processes.

2. Materials and methods

Fig. 1 reports the lab-scale production plant flowsheet.

Tank S1 contains water which equilibrates at room pressure with compressed air, that is bubbled inside the tank. In this tank, at room conditions, water reaches equilibrium solubility of atmospheric gases as verified by the probe oxygen measurements. Degassing unit R1 works at pressure lower than atmospheric so that water enters by depression. Peristaltic pump G1 is used to remove water from degasser. It is a jacketed cylindrical glass container, 350 mm height and with a diameter of 145 mm, in which the working conditions (temperature by a thermostat and pressure by valve V6 and pump G2) are set. The capacity of the degassing unit is about 5 L. The system is kept stirred by a magnetic stir bar. Here takes place the degassing of water. A thermocouple and a manometer gauge the temperature and the pressure of the degassing unit respectively. Pump G2 output is sent to the analysis section in which an online micro-GC previously calibrated analyses the enriched air composition. The gas chromatograph is a micro-GC Agilent 3000A, equipped with a MOLSIEVE column, kept at 45 °C, and a TCD detector. Another manometer measures the line pressure after the pump G2. We sampled the EA every 5 min. The line ends in a Ritter TG01/5 gas meter, used for measuring the amount of EA produced.

The plant is also equipped with a helium line that was used at the start of every experiment in order to purge the system, both the degassing section and the analysis section, from atmospheric air. This procedure was necessary because the air contained in the equipment at the start of the test, if not removed, cause a dilution of the EA produced, this would result in an underestimation of the EA composition and with an overestimation of the volume of EA produced.

We performed 25 experiments changing the three main operating variables, i.e. water inlet flow in a range between 10 and 30 L h^{-1}, degassing pressure between 600 mmHg and 400 mmHg and temperature between 28 °C and 63 °C.

A portable model Hanna Instruments oximeter 9146, equipped with a probe (HI 76407/4F) with compensation of altitude and salinity measured the dissolved oxygen concentration in water after the vessel S1.

Table 1 reports a summary of all the experiments performed, with the operating parameters of each test:

2.1. Simulations

As previously introduced, we modeled the experimental results using the software PRO/II 9.3, developed by SimSci-Schneider Electric, used for the static simulation of chemical processes. Fig. 2 reports a schematic representation of the flowsheet. We modeled

both the vessel S1 and the degassing unit R1 (see Fig. 1) as Flash unit operations (TANK and DEGASSING respectively). In TANK and DEGASSING units, we set the experimental temperatures and pressure values. EA stream pressure was set at 10 atm.

We used the Henry's constants available in the software database (PROII 9.3.EPA) and consider the ideal model for the liquid phase, since the temperature and pressure involved were low and in our system the presence of ions can be neglected. The SRK model was used for the calculation of the vapor entropy.

2.2. Cost analysis

Together with the simulation convergence, we programmed the built-in calculator function in order to calculate the operating and the capital costs (OPEX and CAPEX), according to the Guthrie method (Guthrie, 1969; Guthrie, 1974). Eq. (1) was used for the calculation of CAPEX.

$$CAPEX = C_P^0 * (B_1 + B_2 * F_M * F_P) \tag{1}$$

where C_P^0 is the cost of the module at basic conditions, B_1 and B_2 are the constants for bare module factor, F_M is the material factor for the equipment, F_P is the pressure factor. C_P^0 can be calculated using Eq. (2)

$$\log C_P^0 = K_1 + K_2 * \log A + K_3 * (\log A)^2 \tag{2}$$

in which K_1, K_2, and K_3 are the parameters of the unit operation considered while A the capacity of the unit operation.

F_P can be calculated using Eq. (3)

$$\log F_P = C_1 + C_2 * \log P + C_3 * (\log P)^2 \tag{3}$$

in which C are the constants which accounts for pressurized vessels. In this work, since all the equipment parts work at pressure below 10 bar, all these constants are considered equal to zero.

A summary of the unit operations considered for the CAPEX calculation is reported in Table 2 together with the constants for the cost calculation.

The calculation of the cost of compressor C1 was excluded since it is already included in the compressed air cost. The volumes of the TANK and REACTOR vessels were calculated considering an average water residence time of 0.5 h.

The depreciation time used for the equipment used was 9.5 years and a null salvage cost was assumed for the calculations, according to Turton (Turton et al., 2012). All the costs calculated were actualized to 2013 using the CEPCI index.

The OPEX considered together with their costs is reported in Table 3. All these were considered as provided from off-site (Turton et al., 2012).

Eventually, the enriched air cost was calculated considering a 20 year lifetime for the plant and dividing it by the total volume of EA produced.

3. Results and discussion

3.1. Experimental results

The composition of enriched air versus time and the EA flowrate versus water flowrate are reported in Fig. 3.

The stationary equilibrium value of oxygen concentration was reached for all the tests after about 200 min from the start of the experiment and it depends mainly by operating pressure. All the experimental EA compositions obtained are reported in Table 1. Simultaneously, an increase in temperature (see RUN 3–5) and a decrease in pressure (see RUN 1, 12 and 25) result in a higher percentage of oxygen in EA. With lower operating pressure (see RUN 5–18), stationary equilibrium is reached in lower time, i.e. at