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Research article

Aspen Plus process-simulation model: Producing biogas from VOC emissions in an anaerobic bioscrubber

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A B S T R A C T

A process-simulation model for a novel process consisted of an anaerobic bioscrubber was developed in Aspen Plus®. A novel approach was performed to implement the anaerobic reactor in the simulation, enabling it to be connected to the scrubber. The model was calibrated and validated using data from an industrial prototype that converted air emissions polluted with volatile organic compounds with an average daily concentration of 1129 mgC Nm^{-3} into bioenergy for more than one year. The scrubber, which showed a removal efficiency within 83–93%, was successfully predicted with an average absolute relative error of $5.2 \pm 0.08\%$ using an average height-to-theoretical-plate value of 1.05 ± 0.08 m and 1.37 ± 0.11 m for each of the two commercial packing materials used, respectively. The anaerobic reactor, which treated up to 24 kg of chemical oxygen demand m^{-3} d^{-1} with efficiencies of about 93%, was accurately simulated, both in effluent-stream characteristics and in the biogas stream. For example, the average absolute error between the experimental biogas production and the model values was $19.6 \pm 18.9\%$. The model proved its capability as a predictive tool and an aid in design, resulting in savings of time and money for practitioners. In addition, the approach proposed can be expanded to other bioprocesses that include unit operations.

1. Introduction

Circular economy is attracting more interest from governments, industries, and researchers worldwide. Circular economy is a strategy that attempts to change current linear material- and energy-flow model using a regenerative system in which resource input and waste, emission, and energy leakage are minimized by slowing, closing, and narrowing material and energy loops (Geissdoerfer et al., 2017). The flexographic sector is one field in which the loops could potentially be closed by recycling waste gases into energy. Flexographic industrial facilities, which can consume up to 1000 t of organic solvents per year, produce waste-gas emissions that have relatively low concentrations (below 5 g m^{-3}) of volatile organic compounds (VOCs), mainly ethanol, ethyl acetate, isopropanol, n-propanol, 1-methoxy-2-propanol, n-propyl acetate, 1-methoxy-2-propyl acetate, acetone, and 1-butanol (Granström et al., 2002). Today, these emissions must be treated to follow the European Directive 2010/75/EU (European Council, 2010). However, recently, a novel process, anaerobic bioscrubber, has offered a circular economy approach that enables these emissions to be transformed into bioenergy (Waalkens et al., 2015). In a previous work (Bravo et al., 2017), an on-site anaerobic bioscrubber installed in a flexographic facility was operated for 484 days, controlling VOC emissions that had an average daily concentration of 1129 mgC Nm^{-3}. The VOC removal efficiency at the scrubber ranged from 83–93%, and the anaerobic reactor showed excellent performance, treating organic loading rates (OLRs) of up to 24 kg of chemical oxygen demand (COD) m^{-3} d^{-1} with efficiencies of about 93% and producing a biogas stream that had methane content of 94 ± 3 %vol. This experimental study was the first to demonstrate the potential of this new biotechnology, although more in-depth knowledge of it is necessary to provide an optimized system.

Models are considered useful tools to improve knowledge of bioprocesses, to study their responses against variations in parameters, and to predict their overall performance (Okkerse et al., 1999; Zarook et al., 1997). In fact, process simulators are highly

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appreciated by industries and researchers because they can perform accurate predictions and sensitivity analyses in less time and much less expensively than can be done in real plants (Al-Rubaye et al., 2017; Rajendran et al., 2014), thereby aiding process design and optimization. One of the most powerful process simulators is Aspen Plus®, an integrated process engineering software program that performs steady-state and dynamic-process simulations. The software includes equipment-design and cost-evaluation tools and incorporates rigorous property methods, thermodynamic calculations, and the ability to use electrolyte equilibriums and a wide range of unit operations.

Regarding the application of simulators to the main unit operations of anaerobic bioscrubbers, Aspen Plus® is an established tool for simulating and making predictions about absorption systems (Azahari et al., 2016; Bhoi et al., 2015; Sutanto et al., 2017). Regarding the modeling of anaerobic digestion processes, the Anaerobic Digestion Model no.1 (ADM1), proposed in 2002 (Batstone et al., 2002), is considered the most advanced model for predicting, controlling, and optimizing the production of biogas using anaerobic digestion processes. The ADM1 includes biochemical processes, including disintegration, hydrolysis, acidogenesis, acetogenesis, and methanogenesis, and physicochemical processes, including gas-liquid equilibriums and ion dissociations. Some extensions to the ADM1 have been proposed (Batstone et al., 2006), and the model has been used by a number of researchers to simulate various types of biogas-production processes from different substrates for both labs and full-scale biogas plants (Hagos et al., 2017).

However, the complexity of the ADM1 model, with its large numbers of components, has led to the application of both simplified versions of the model and to simpler models (Arzate et al., 2017; Kleerebezem and Van Loosdrecht, 2006). Indeed, the few available studies on the implementation of anaerobic digestion in Aspen Plus® have used simplified approaches to the anaerobic-digestion model. For example, Barta et al. (2010) conducted a techno-economic evaluation of stillage anaerobic treatment in a softwood-to-ethanol process. The author assumed stoichiometric degradation factors of 90% for soluble compounds, 50% for polysaccharides and water-soluble lignin, and 0% for nonsoluble lignin, with a yield of 0.35 Nm^3 kg COD^{-1} for methane production. Nguyen et al. (2014) used the theoretical stoichiometric method based on the Buswell equation to evaluate the products of the anaerobic digestion of food waste for their energy potential. Salman et al. (2017) techno-economically evaluated biomethane production by integrating pyrolysis and anaerobic-digestion processes, using stoichiometric factors for the methane produced from carbohydrates, protein, and lipids. Rajendran et al. (2014) and Al-Rubaye et al. (2017) proposed a similar approach using Aspen Plus® reactor blocks connected in series. Both studies defined the hydrolysis step in a stoichiometric reactor, using different conversion grades for carbohydrates, proteins, and lipids; whereas the acidogenesis, acetogenesis and methanogenesis steps were carried out in continuous stirred tank reactors, defining the degradation kinetics in a homemade calculator block.

The purpose of the present study was to develop a process-simulation model of the anaerobic bioscrubber that would be a useful tool for optimization and design. The simulation model was calibrated and validated using experimental data obtained in a previous study, in which a prototype of anaerobic bioscrubber was operated during 484 days (Bravo et al., 2017). The two main process units, the scrubber and the anaerobic reactor, were created in Aspen Plus®, which is capable of defining the gas-liquid equilibriums and the electrolyte chemistry. The anaerobic degradation reaction kinetics of the acidogenesis and methanogenesis steps were assumed as Monod-type expressions. This article includes the assumptions used to implement the anaerobic bioscrubber in Aspen Plus®. In addition, a sensitivity analysis evaluated the effect of the model's parameters on the predictions of both units. Finally, a case study showed the model's capability as a design tool.

2. Materials and methods

2.1. Anaerobic bioscrubber prototype

The process-simulation model developed in this study was calibrated and validated using data obtained previously from an anaerobic-bioscrubber prototype installed on-site in a flexographic printing facility. This system was successfully operated for 484 days to control VOC emissions that were mainly composed of ethanol (ET), ethyl acetate (EA), and 1-ethoxy-2-propanol (E2P) (Bravo et al., 2017). The anaerobic bioscrubber consisted of two interconnected units: a scrubber of 2.0 m in packing-material height and 0.5 m in diameter that was assembled onto a 2-m^3 tank and an expanded granular sludge bed anaerobic reactor having a diameter of 1.59 m and a total water volume of 8.7 m^3. The reactor was filled with 3 m^3 of granular sludge. Fig. 1 shows a scheme of the prototype. The flexographic site runs two 8-h shifts each day from Monday through Friday and one 8-h shift on Saturday. A fraction of the VOC emissions from the factory was blown into the scrubber, flowing counter-currently to a water stream. The airflow of this fraction varied from 184–1253 $m^3\ h^{-1}$, and the average daily VOC concentration was 1129 ± 460 mgC Nm^{-3}. The water stream containing the solvents from the scrubber tank was supplemented with sodium carbonate for pH control and macro- and micronutrients prior to flowing into the anaerobic reactor, which operated at 3 h of hydraulic residence time. The effluent from the reactor was sent to the scrubber unit, meaning that the pilot plant worked in water-closed recirculation. During the study, three different scrubber configurations were tested in the plant, as follows: 1) a cross-flow structured packing material (KFP 319/619, ENEXIO, Germany, named Packing A) was used from days 0–95 (Stage I) and from days 266–484 (Stage V); 2) a vertical-flow structured packing material (KVP 323/623, ENEXIO, Germany, named Packing B) was used from days 96–130 (Stage II) and from days 181–265 (Stage IV); and 3) a spray column was used from days 131–180 (Stage III). More information of the commercial packing materials can be found in supplementary section. Several liquid-to-air volume ratios ranging from 1.9×10^{-3}–10.1×10^{-3} were set in the scrubber unit, resulting in superficial liquid velocities of from 10.2 to 20.4 m h^{-1}. The organic load (OL) fed to the anaerobic reactor fluctuated according to modifications in the facility and the operation of the scrubber and ranged from 0.37–6.96 kg COD h^{-1}.

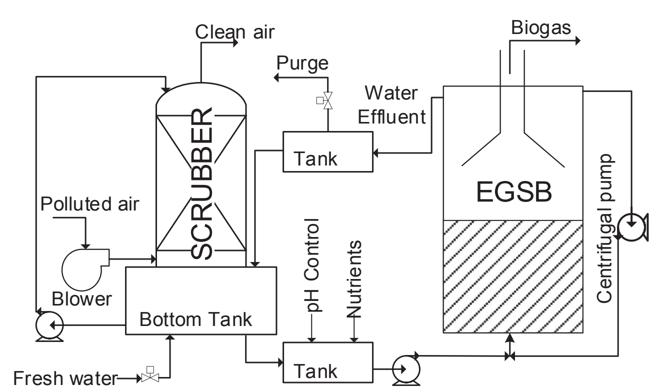

Fig. 1. Scheme of the anaerobic bioscrubber prototype.

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