Aspen Plus designing and optimizing the hospital wastewater treatment by wet air oxidation method

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Abstract. Healthcare establishments, pharma industries, and medical laboratories generate various waste materials, collectively called hospital or healthcare waste. Waste management regulations differ depending on the laws and acts adopted by the authorities and their level of compliance. For instance, in the United States of America, hospitals follow the rules set by the European Environmental Protection Agency. In Europe, hospitals adhere to guidelines and standards set by the European Environmental Agency, while globally, the World Health Organization has established standardized policies and regulations. As a result, waste treatment technologies have become more prevalent for making medical waste non-infectious. These treatments include thermal treatment using microwave technologies (e.g., Wet air oxidation), steam sterilization, electropyrolysis, and chemical and mechanical systems. This research aims to model the treatment of hospital wastewater by wet air oxidation method using Aspen Plus for the first time in Lebanon. The simulation showed that the reaction conversion yield for thiols or mercaptans was 89.7% and 83.8% for sodium hydrosulfide, and the COD and BOD5 levels were reduced by 79.1% and 88%, respectively.

1 Introduction

Healthcare establishments, pharma industries, and medical laboratories produce different types of waste, collectively called hospital or healthcare waste [1]. This includes the waste produced during healthcare procedures at home, such as dialysis and insulin injections. Waste management regulations differ depending on the laws and acts adopted by the authorities and their level of compliance. For instance, in the United States of America, hospitals follow the rules set by the Environmental Protection Agency (EPA) [2], which has established strict emission standards for medical waste [3]. In Europe, hospitals adhere to guidelines and standards set by the European Environmental Agency (EEA) [4], while globally, the World Health Organization (WHO) has established standardized regulations and policies [5]. As a result, waste treatment technologies have become more crucial for making medical waste non-infectious and less damaging to the environment [3]. These treatments include steam sterilization, thermal treatment using microwave technologies (e.g., Wet air oxidation), electropyrolysis, and chemical and mechanical systems.

1.1 Healthcare waste

Hospital or healthcare waste can be classified into several categories based on the types of waste generated in healthcare facilities and their potential hazards. The classification of healthcare waste varies across different countries and regions, but the following categories are commonly recognized:

- Infectious waste: WHO defines infectious waste as the waste contaminated with blood or other bodily fluids, as well as waste from patients with infectious diseases such as COVID-19, HIV/AIDS, hepatitis B and C, and tuberculosis [6].
- Pathological waste: it includes human tissues, organs, and body parts, as well as animal carcasses and other waste produced during surgical procedures, autopsies, and research [7].
- Sharps waste: it includes needles, syringes, lancets, scalpels, and other medical instruments that can puncture the skin and pose a risk of infection or injury [7].
- Chemical waste: it includes discarded chemicals, such as disinfectants, solvents, and laboratory reagents [7].
- Pharmaceutical waste: it includes expired or unused medicines, as well as chemotherapy drugs and other hazardous pharmaceuticals [8].
- Radioactive waste: it is the waste contaminated with radioactive materials, such as diagnostic and therapeutic equipment used in nuclear medicine.

1.2 Healthcare Waste in Lebanon

In Lebanon, the amount of waste generated per hospital bed is estimated to be higher than the global average by about 1.7 kg, at 5.7 kg/bed/day [9, 10]. Despite this,

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Lebanon has achieved a high ranking in Bloomberg's Healthcare Efficiency Index, placing 23rd worldwide in medical services with a score of 53.0 for efficiency, a life expectancy of 79.4 years, and a relative cost of 7.4% [11]. Factors contributing to the ranking of each country are emergency response time, available surgical procedures, residency time, and hygiene. In terms of hygiene and cleanliness, Lebanese hospitals scored an average of 4.32 out of 5 for sanitation, sterility, hygiene, and cleaning guidelines, according to the Lebanese Ministry of Health [12].

Considering the above facts and figures, untreated wastewater has a catastrophic environmental impact. In particular, treating hospital wastewater is essential as it is well known to be a pool of toxic/nonbiodegradable/infectious pollutants. Moreover, hospital wastewater has high chlorides and surfactants, moderate organic compounds (e.g., E. Coli), moderate BOD, and high COD levels [13]. As a result, proper hospital wastewater treatment is crucial in the Lebanese context since the country lacks sustainable development plans for waste management.

1.3 Wastewater treatment by wet air oxidation

Wet air oxidation (WAO), also known as thermal liquidphase oxidation, is a wastewater treatment process that uses high temperatures (150°C to 320°C) and pressurized (10 to 220 bars) air or oxygen to oxidize toxic substances and hazardous materials [14]. During this process, hydroxyl radicals are produced. These radicals are known for their high oxidizing properties, fast decay rate and reactivity, and excellent affinity for consuming toxic substances [15]. The resulting products are either partially degraded or mineralized into biodegradable intermediates such as H₂O, CO₂, and inorganic salts. Furthermore, catalysts (e.g., Hydrogen Peroxide) can be incorporated to enhance reaction rates and efficiency. Wet air oxidation technologies significantly decrease the high organic load in hospital wastewater due to their high affinity to dissolve organic matter. WAO, represented by a flow diagram (Fig. 1), consists of a continuous rotary compressor and pumps that compress the air or oxygen and feed the liquid stream to the required operating pressure [16].



Fig. 1. Typical wet air oxidation system.

Heat exchangers recover the energy from the reactor effluent and preheat the feed entering the reactor. The

residence time in the reactor vessel for several hours at sufficient temperatures and pressures allows adequate mineralization and biodegradability of toxic substances in the wastewater reaction tank. Naturally, oxidation reactions are exothermic, considerably cutting off different heat needs for continued operation at COD levels of 10000 mg/L or above [17,18].

For the first time in Lebanon, this research aims to design and optimize an effective, reliable, and sustainable wet air oxidation treatment process for Lebanese hospital wastewater using Aspen Plus software.

2 Methodology

Aspen Plus software (version 11) simulates and optimizes the wet air oxidation treatment process for Lebanese hospital wastewater based on the model developed by Siemens [14-16]. Building the flowsheet begins by entering the chemical components needed throughout the model. Oxygen, nitrogen, water, methyl mercaptan, dimethyl disulfide, sodium hydroxide, sodium sulfate, and air are used for the wet air oxidation process. The following step is adding the property method. This step is crucial to the successful and correct convergence of the model. The case of the wet air oxidation treatment process simulation, the SRK property method was used. Afterward, blocks (e.g., reactors, compressors, pumps, mixers, etc.) and streams (e.g., feed, entry and exit streams, etc.) are fixed within the simulation environment. The last step of building an Aspen Plus model is to enter the required inputs for the blocks and streams already added to the primary flowsheet. This step sets operating conditions such as temperature, pressure, flow rates, mass or mole fractions, number of stages, etc. Our model modeled the wet air oxidation process using air as an oxidizing agent without any catalyst. In this case, the temperature required for a chained induction period and the high free-radical count were set to 320°C while the reactor's pressure was fixed at 220 bars. It is worth mentioning that the higher the temperature applied, the higher the pressure is required to avoid converting the mix into the gaseous phase. The required input of specific blocks and their stream results are shown in Figures 18 to 21, while Figure 22 depicts the input for each block.

To optimize and improve our model, three alternatives were considered:

- Control and stabilize the sodium sulfate while varying the wastewater and oxygen feeds.
- Detract dimethyl sulfoxide to the off-gas byproducts while achieving a sufficient flash separator operating temperature.
- Use of ultrasonic probes in the reactor.



Fig. 2. Flowsheet of the Wet Air Oxidation process (S1-S9 represent the streams).

3 Results and discussions

The critical input and simulation output data results are presented in Table 1 below. The table shows that the reaction conversion yield for thiols or mercaptans was 89.7% and 83.8% for sodium hydrosulfide, with a deviation lower than the margin error suggested in Siemens' experimental methodology (5%). Our results align with the ones of S Chandraseagar et al., where the developed and validated Aspen Plus model for fractional conversion of NaHS and mercaptans has a difference of less than 5% between the simulation result and the published experimental data [14]. As a result, the model was successfully considered to approximate the actual system and provided a base for further improvement. Additionally, the levels of COD and BOD5 were reduced by 79.1% and 88%, respectively.

Table 1. Simulation results in Aspen Plus.

Temperature	Pressure	Time	
(°C)	(bar)	(hour)	
140.00	3.00	0.67	

		Feed	Off-gas
Mass Flow Rate	Litre/hr	828.13	46.2
Oxygen	Litre/hr	0	0.0074
Nitrogen	Litre/hr	0	8.4340
Water	Litre/hr	823.4	37.19
Methane thiol	Litre/hr	0.3682	0.03792
Dimethyl disulfide	Litre/hr	0	0.314
Sodium Hydroxide	Litre/hr	2.15	5.1e-15
Sodium sulfate	Litre/hr	0	0.0009
Sodium hydrosulphide	Litre/hr	2.15	0.3494
COD	mg/L	450	94.05
BOD5	mg/L	290	34.6

3.1 Optimum Ratio of HWW Feed Flow Rate to Air Flow Rate

To optimize the wet air oxidation treatment process, the airflow rate in Aspen Plus was adjusted in seven simulation runs while maintaining a constant flow rate of HWW. The success of each run was determined by monitoring the decrease in sodium sulfate (Na₂SO₄) over the simulations. When a consistent conversion output for Na₂SO₄ was achieved, it was concluded that the HWW feed-to-air feed ratio had reached an optimal value of 1:9.2. Figure below illustrates the relationship between Na₂SO₄ and the amounts of HWW and air used. It is

important to note that the air should contain excess oxygen to ensure that oxidation is completed in the reactor.

The Figure below depicts the changes in Na_2SO_4 as a function of the quantities of HWW and air used. It should be emphasized that the air fed into the reactor must contain excess oxygen to ensure the oxidation process is fully completed.



Fig. 3. Evolution of Na_2SO_4 versus the amounts of HWW and airflow rates.

3.2 Optimum operating temperature of the flash separator unit

Once the oxidation reactions have been optimized, the temperature of the flash separator needs to be adjusted to achieve maximum separation of dimethyl disulfide (DMDS) due to its high volatility and toxicity, even in small amounts. During simulation runs, the pressure was maintained at 3 bars while the operating temperature was manipulated. The optimum temperature for the flash separator was assumed to have been reached when the DMDS levels became stable with no further change. Figure 4 displays the changes in DMDS levels as a function of the varying temperatures of the separator.



Fig. 4. Evolution of DMDS regarding the varying operating temperature of the flash separator.

4 Conclusion

The treatment of hospital wastewater through wet air oxidation was simulated using Aspen Plus software, with the model subsequently optimized to improve overall yield and power consumption. The simulation results, including organic loads, sodium hydrosulfide, COD, and BOD5 levels and yields, were validated against data from published articles. The simulation achieved a deviation below 5 percent, indicating its success. The optimized operating conditions for the reactor and flash separator were determined to be a ratio of 9.2 to 1 (air to HWW) and a temperature of 140°C, respectively.

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