**Simulation-based design of a bipolar membranes electrodialysis unit for chemicals production from brines.**

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**1.Introduction**

Nowadays environmental concerns are modifying the production and consumption patterns used so far. An important objective to improve our society is the use of sustainable processes that can reduce industrial waste streams. Bipolar membranes electrodialysis (EDBM) is an emerging environmentally friendly process that could be easily integrated into a circular economy approach to valorize waste brines. It is an electro-membrane process that allows the production of chemicals using only water, electrical energy and a salty solution. When electric current is applied to the electrodes of the EDBM stack, water dissociation takes place in the bipolar membranes. Therefore, the ions from water are combined with those coming from the salt generating acid and base. The increasing interest in the EDBM process requires appropriate design procedures. This study proposed a simulation-based design of a EDBM unit for the production of hydrochloric acid and sodium hydroxide from sodium chloride solution. The design was performed in terms of configuration and operational conditions. A model, realized by Culcasi et al. [1], was used to describe the EDBM process’s behaviour. This model was validated with experimental data so that a high quality design could be achieved. This procedure was used to design a EDBM unit that will be part of the demo-plant of the Horizon 2020 Water-Mining project.

**2. Methods**

To properly design the EDBM unit it is important to define the initial conditions of the process, in terms of concentrations and volumes of the of the three solutions (acid, base, salt) fed to the EDBM unit and the target concentration at which stops the process. Then, it is important to select a specific type of membranes and spacers with dimensions appropriate to the scale of the process. To take into account the resistance of the electrode compartments, the Blank resistance is needed; this could be calculated in the laboratory or taken from literature. It is also necessary to define some configurations that will be investigated to find out which is the most appropriate. The procedure uses only three performance parameters: process time, Specific Energy Consumption (SEC) and Specific Production (SP). These three parameters will be monitored in the simulations of the selected configurations and then used to select which is the best. The SEC is the energy consumed to produce 1 kg of the target product and it is expressed in *kWh/kg*. The SP is the flowrate of target product produced by one triplet with a unit membrane area and it is expressed in *kg/(h m2triplet).*

The EDBM unit of the Water-Mining will be operated in closed-loop (batch way) in order to reach high concentration of electrolyte solutions. The initial conditions of the three solutions fed to EDBM unit and the target that we want to reach at the end of the process are reported in Table 1.

**Table 1.** Initial conditions of the three solutions fed to the EDBM unit and target that we want to reach at the end of the process.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ***Solution*** | ***V0 [m3]*** | ***C0,NaCl [mol/l]*** | ***C0,NaOH [mol/l]*** | ***C0,HCl******[mol/l]*** | ***TargetNaOH******[mol/l]*** |
| *Acid*  | *0,5* | *0,01* | *-* | *0,02* | *-* |
| *Salt* | *0,5* | *2* | *-* | *0,01* | *-* |
| *Base*  | *0,5* | *0,01* | *0,02* | *-* | *1* |

The membranes selected for this EDBM unit are fumasep® FAB, FKB, FBM as anionic, cationic and bipolar membrane respectively. Six different configurations were selected with a total number of triplets that ranges from 20 to 60 that could be disposed in one or two different stacks arranged in a parallel way. The configurations were simulated at three different current densities, 200, 400, 600 A/m2.

**3. Results and discussion**

The results of the simulations are reported in Figure 1. With the same total number of triplets, the time reduces if two stacks in parallel are used. The SEC, plotted as a function of the number of triplets in one stack, shows a trend with a minimum. The minimum always lies between 20 and 30 triplets in one stack. There is also an increase in the SEC with the increase of the current density. Focusing on the SEC, it is convenient to use a number of triplets that range between 20 and 30 in one stack and a low current densities. The SP shows a monotonous decreasing trend as the number of triplets in one stack increases; it also increases linearly with the current density. From the point of view of the SP, it is convenient to use a low number of triplets in one stack and a high current densities. Taking into account all these parameters, in order to minimize the time and the SEC and maximize the SP, the best configuration is that with a total number of triplets equal to 40, arranged in two stacks in parallel. This configuration needs to be operate at moderate current density (400 A/m2).

 

**Figure 1.** a) Process time, b) Specific energy consumption and c) Specific production for the configurations analyzed at three different current densities.

The procedure’s results were compared to those obtained from a cost-of-production analysis of sodium hydroxide. The cost was calculated as the sum of CAPEX and OPEX. The analysis demonstrates which values of triplets number and current density minimize production cost. It was found that a number of triplets of 44 and a current density of 300 A/m2 are the values that minimize the cost of sodium hydroxide production. It can be seen that those values are very similar to those obtained with the proposed procedure.

**4. Conclusion**

This work presented a procedure for designing an EDBM unit. The unit was simulated with a model that was validated with experimental data. Three important performance parameters, that take into account the main aspects of these units, were used to carry out the design. The results of the procedure were compared with those from a cost-of-production analysis, thus demonstrating the design’s efficacy.

**5. Acknowledgement**

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**References**

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