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Methodology to optimize fluid-dynamic design in a redox cell

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HIGHLIGHTS

- Methodology proposed based on CFD, for optimizing redox cells design.
- Parameters definition: quantifying uniformity and symmetry of electrolyte velocity.
- Numerical techniques applied to velocity analysis (CFD and Hypothesis test).
- Case study using the methodology, defining an optimized redox cell geometry.

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ABSTRACT

The present work is aimed at the optimization of a redox cell design. The studied redox cell consists on a device designed to convert the energy of reactants into electrical energy when a liquid electrolyte reacts at the electrode in a conventional manner. In this particular sort of cells, the two electrolytes are present and separated by a proton exchange membrane. Therefore, the flow of the electrolyte and the interaction with the membrane takes a paramount importance for the general performance of the cell. A methodology for designing the inlet part of the cell based on optimizing the uniformity of the flow and the initial position of the membrane is presented in this study. This methodology, based on the definition and optimization of several parameters related to the electrolyte flow in different regions of the geometry, is depicted. The CFD (Computational Fluid Dynamics) model coupled with the statistical study pointed to several practical conclusions on how to improve the final geometry construction of the redox cell. A particular case study of redox cell is implemented in order to validate the proposed methodology.

1. Introduction

Redox Flow Cells are large stationary electricity storage systems. This sort of energy storage technologies will play a paramount role in the near future. The increasing use of efficient energy sources and renewable energy such as wind and solar, makes them necessary. These technologies usually suffer from experiencing intermittent generation [1] and the storage of energy is crucial to avoid the intermittency in the supply system.

The leading edge research impulses the development of energy storage to release the consumer system needs [2–4]. On a large scale, this energy storage could alleviate the unpredictability of energy sources to promote their accumulation over time [5].

Among these technologies, one of the most prominent is the redox flow battery (RFB). It is one of the best options for energy storage at medium and large scale [6]. The performance of these batteries is based on storing energy in solutions containing different redox couples. The electrodes surface makes possible the reversible electrodic processes. Redox and semi-redox technologies are good candidates for large stores of energy and medium domestic use storage, respectively [7].

On the one side, in this sort of batteries, the accumulated electrolyte determines the amount of energy stored. On the other side, the battery power depends on the electrode surface. The power stage is directly related to the active mass of the electrode, as the energy storage [8].

Accordingly, such batteries can modulate their output voltages and storage capabilities, and multiple cells can be interconnected using different sized reservoirs. Furthermore, they are very adequate as potential energy storage systems for distributed generation. In such cases the needs of each system determine their own requirements.

One of the first documented works on the redox flow cell was presented by Thaller in mid 1970s [9]. Since then, the redox flow cell concept has been implemented in different strategies, materials and chemical alternatives [10]. The numerically analysis of flow of electrolyte makes sense with the development of Computational Fluid Dynamics Technology (CFD), considering the precursors

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described in the papers of Frías-Ferrer [8] and Codina [11] Weber et al. 2011 [7] compile an interesting summary of Redox batteries. In these research conclusions it is highlighted that the future of this technology goes through optimizing designs modeling, both: flow and transport. In this sense, different materials have been applied in redox batteries, with different geometries [6,7,12].

Fig. 1 shows the scheduled diagram of a redox cell. The two cylinders placed on the sides of the figure represent the two electrolyte storage tanks. The tank on the negative electrode storages a redox solution, this solution will be different from the tank on the positive electrode. There are two pumps, one on each side of the reactor (Fig. 1). These pumps force the flow to circulate through the electrolyte in order to allow the semi-occurring redox reactions involving transfer of load.

The cathode is made of graphite of carbon felt. The anode is also made of graphite or carbon felt with a selective membrane as separator. The membranes are made up of cross-linked linear polymer chains, which form a three-dimensional network. Without the cross-linking, the membrane would be dissolved in water forming a polyelectrolyte solution. Ion exchange membranes have fixed ion functional groups and oppositely charged counter ions, present in sufficient numbers to render the whole exchanger electrically neutral. The reactions achieved in the cell (considered as an all-iron redox cell) are:

- $2Fe^{2+} \rightarrow 2Fe^{3+} + 2Fe$, during the charge
- $2Fe^{3+} + 2Fe \rightarrow 2Fe^{2+}$, during the discharge

The electrolyte composition for this purpose is 2 M $FeCl_2$ + 0.5 M NH_4Cl in deionized water, as based on [13]. The working temperature is 40 °C, the fluid viscosity at this temperature is $1.143 \cdot 10^{-3}$ (Ns m^{-2}). It has been assumed that the electrolytic fluid produces no deposition within the cell as well as it does not produce any gas phase. This hypothesis would be completely true if the redox reaction was 100% efficient. In reality, other competing reactions can occur with little gas production; these are disregarded as hypothesis [14]. Another assumed hypothesis is the one concerning the fluid density. Density is considered constant (1172 g m^{-3}) for all kind of flow.

The cell structure is surrounded by bipolar plates composed by structural support and electrical conductor. The electrodes, located on the side of each bipolar plate, are not involved in the electrochemical reactions. Nevertheless, they are important as they provide a surface facilitating the electron path. The membrane is located between both sides of the reactor. The membrane separates the two electrolytes, in order to preserve the electro-neutrality. The so considered volume 'A' (Fig. 1) is occupied by electrolyte. In this paper, the interest is focused on the uniformity of the electrolyte flow along this 'A' volume. Only the flow in the positive side of the cell is analyzed, as a symmetrical geometry is presented for both sides of the cell (positive and negative).

The uniformity of flow has a significant influence on the most important parameters of performance in the cell: the effective area of the electrode; the strength and efficiency; the useful life of the battery and electrochemical polarization (particularly under high current density variation [15]).

The consulted references propose that the flow of electrolyte through the active layer has a high inference performance thereof [16]. In 1998, Moyabayashi et al. [17] concluded that the increase in energy efficiency is essentially determined by a uniform distribution of electrolyte. However, although the flow is homogeneous, there could be significant local variations in the surface of the electrodes, among others, causing strong changes of pH. Furthermore, the interest between different geometries and flow conditions in different redox cells have been considered in the literature, focused on understanding and improving the functioning of the whole reactor [18–21] and the membrane position and configuration within the whole geometry [22].

Due to the fully compact battery system, the use of completely opaque key materials and the strong acidity of the electrolyte, the fluid distribution within the battery is often difficult to be determined, measured and quantified. However, the consulted references agree that research is vital to determine the optimal functioning of the battery pack [23,24].

Thus, the strategies for redox cell design should pay the most interest in the analysis of the velocities at all points of the trajectories of the fluid. It is especially interesting in the inlet part of the cell [25]. Nevertheless, an exhaustive treatment of these flow fields, especially in the design phase, requires two important numerical tools: on the one hand, Computational Fluid Dynamics (CFD) and on the other hand, statistical techniques. The use of CFD will help designers to simulate the velocity and pressure fields in the

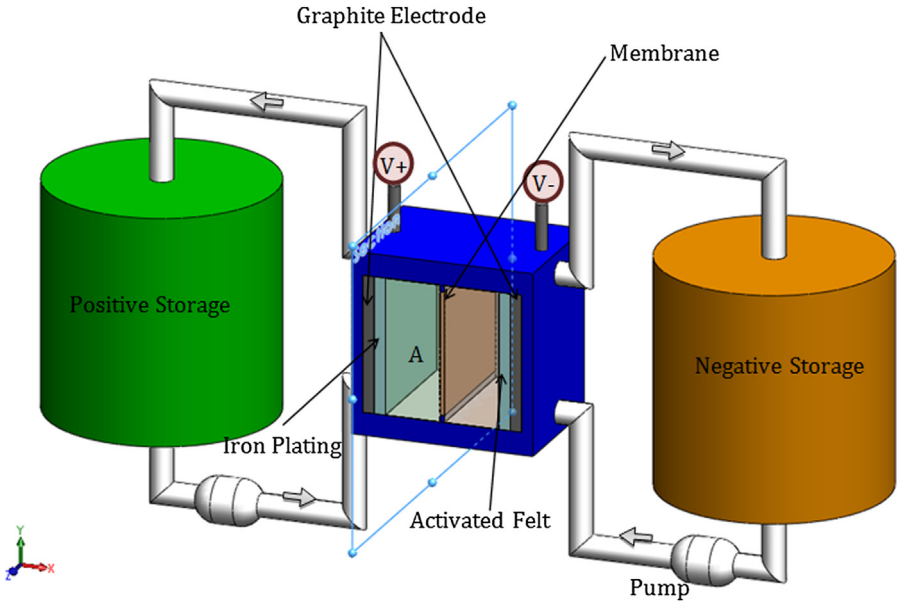

Fig. 1. Diagram of an iron flow battery (system components).