Abstract

This thesis proposes the use of a methodology that estimates the importance of the electrolyte flow hydrodynamic optimization in electrochemical reactors with experimental validations. This methodology is based on the computational fluid mechanics modelling.

Through the set up and analysis of some indicator parameters, the research described here will allow the implementation of improvements to optimize in a feasible way the current designs of the reactors' cells.

Therefore, the aim of this thesis is to analyse and reveal the different flow paths of the electrolyte inside the chemical reactor through the use of a numerical code that solves the electrolyte fluid mechanics in the proposed geometries. This approach allows, on the one side, to determine some quantifiable parameters which analyse the kindness of the designs in order to obtain flow visualizations and, on the other side, to obtain quantifiable parameters that allow possible optimization designs. The proposed design and parameters are experimentally validated in two different geometries made for that purpose.

This general objective could be subdivided in a series of more specific objectives, which are detailed as follows:

- Study the economic viability based in the Spanish market of this kind of batteries.
- Analyse in depth researches carried out up to now on CFD techniques (Computational Fluid Dynamics) optimisation of the flow channels inside the electrochemical reactor, either through functional methodologies or through other design techniques.
- Evaluate the goodness of the different developed CFD models compared to experimental models, with special attention to the feasibility of the computational model results compared with the physical ones.
- Propose our own parameters in order to quantify the reactor efficiency, based on flow velocity inside the cell.
- Define the best adjustment of the diverse design operators for each of the optimization proposals.

- Obtain an optimal geometry based on the design parameters for the full scale construction cell.

From the proposed methodology, an optimization protocol has been followed regarding the final influence of the electrolyte flow inside the cell.

The developed analysis proves the capital importance in the Spanish energetic sector of the energy storage devices proposed in this thesis. An economic analysis of a particular cell shows that such a battery is economically viable, estimating a return of investment in between 8 to 9 years.

As well, a validated model of an experimental prototype has been developed with lab measurements and numeric simulations that lead to believe that the use of computational fluid dynamics is valid.

Through the use of the commercial software STAR-CCM+ from CD-Adapco$^©$, we have validated an initial scaled down prototype in use at the Electrochemistry Department of the Universidad de Alicante (Spain). This validation gives a mean error of 2.22 % and has estimated some working parameters, such as the fluid volume that circulates along the main flow direction, being this one of an 83 %.

In this thesis, a joint methodology is proposed, based on the obtained experience in the previous phases according to the following concepts: symmetry coefficient, uniformity coefficient, variability range coefficient and rate of fluid circulating in the main direction.

The symmetry coefficient indicates the circulating flow rate difference through each of the two sides of the cell in the longitudinal direction. The uniformity coefficient evaluates the average velocity in the channel. The variability range coefficient analyses the velocity of the fluid in a specific point of the membrane in order to determine the velocity variability. Finally, the defined volume flow in the main direction estimates the laminarity and direction of the flow inside the cell. This methodology is used to optimize the battery by modifying pre-existent dispositions, obtaining a final geometry in which the number of channels before the membrane is 84, with an interchannel separation of 1 mm, validated with experimental pressure and velocity measurements in a prototype at the Justo Nieto mechanical fluids laboratory in the Polytechnic University of Valencia which allows to confirm the purpose numerical model.

The developed battery shows an improved design regarding previous designs. The battery has a perfect symmetry and a uniform distribution when the fluid reaches the membrane with a nearly null volume of circulation in the membrane zone. This battery validates the proposed methodology for the design of this type of elements based on the flow mechanics of the electrolyte inside it.

This thesis includes a conference communication and four articles published in peer reviewed journals indexed in the "Journal Scitation Reports" as detailed below.

- Escudero González, J.; Alberola, A.; López Jiménez, P.A. 2012. Computational Fluid Dynamics Applied to a Prototype Flow Battery. III International Flow Battery Forum (IFBF 2012). Munich, June de 2012. Minutes Book. Pages 14-16. ISBN 978-0-9571055-2-2.

- Escudero Gonzalez, J.; Alberola, A.; López-Jiménez, P. A. 2013. Redox Cell Hydrodynamics Modelling. Simulation and Experimental Validation. Engineering Applications of Computational Fluid Mechanics. Volume 7. N 2. Pages 168-181. June 2013. (journal impact factor in 2012: 1.144; Q2).

- Escudero-González, J.; López-Jiménez, P. A. 2014. Methodology to Optimize Fluid-Dynamic Design in a Redox Cell. 2014. Journal of Power Sources. Volume 251, 1 April 2014, Pages 243–253. (journal impact factor in 2012: 4.675; Q1)

- Escudero-González, E.; López-Jiménez, P.A. 2014. Iron redox battery as electrical energy storage system in the Spanish energetic framework. International Journal of Electrical Power & Energy Systems. Volume 61, October 2014, Pages 421–428. (journal impact factor in 2012: 3.432; Q1)

- Escudero-González, J.; López-Jiménez, P.A. It is awaiting publication. Redox Cell Hydrodynamics Modelling. Towards a Real Improved Geometry based on CFD Analysis. Article in press, accepted for publication in Engineering Applications of Computational Fluid Mechanics. (Journal impact factor in 2012: 1.144; Q2).