Slovak Society of Chemical Engineering
Institute of Chemical and Environmental Engineering
Slovak University of Technology in Bratislava

PROCEEDINGS

51st International Conference of the Slovak Society of Chemical Engineering SSCHE 2025

Hotel DRUŽBA

Jasná, Demänovská Dolina, Slovakia

May 27 - 30, 2025

Editors: Assoc. Prof. Mário Mihaľ

ISBN: 978-80-8208-158-2, EAN: 9788082081582

Published by the Faculty of Chemical and Food Technology Slovak Technical University in Bratislava in Slovak Chemistry Library for the Institute of Chemical and Environmental Engineering; Radlinského 9, 812 37 Bratislava, 2024

Blahušek, V., Gráf, D., Staś, J., Bureš, M., Zubov, A., Mazúr, P.: Modelling metal deposition on a 3D electrode in a hybrid flow battery: Validation by microcomputed tomography imaging, Editors: Mihaľ, M., In *51st International Conference of the Slovak Society of Chemical Engineering SSCHE 2025*, Jasná, Demänovská Dolina, Slovakia, 2025.

Modelling metal deposition on a 3D electrode in a hybrid flow battery: Validation by microcomputed tomography imaging

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Key words: Hybrid redox flow batteries, modelling, micro-computed tomography

While a number of subtypes of redox flow batteries (RFBs) have already been successfully commercialized, hybrid flow batteries (HFBs) still have unresolved challenges. The main difference, setting this subtype apart from most RFBs, is that deposition of metal is required at one of the electrodes. The common issue is, that the metal deposition is uneven across the electrode. This can lead to a host of performance issues, lesser areal capacity during cycling and in some cases even mechanical damage to the cell, shortening its lifespan. To address these issues, mathematical modelling can be employed. It can be powerful tool for understanding the complex process of metal deposition and optimization of the operating parameters of HFBs, which could lead to more uniform deposited metal distribution. However, validation of such model is challenging.

To address this issue, we have developed a macro-homogenous model, which is able to predict the dynamic evolution of the deposited metal distribution. We subsequently validated the model predictions using online pressure drop and conductivity measurements as well as spatial metal distribution obtained from imaging techniques, including 3D micro-computed tomography. The model is based on a zinc-iodine hybrid flow battery with a 3D porous negative electrode. In the proposed model, the 3D electrode is characterized by locally distributed porosity and conductivity which evolve in time along with the amount of deposited metal. Experimental data (felt electrode compression rate, current flow, pressure drop) and 3D micro-computed tomography porosity estimates, all sourced from our previous papers [1, 2], were used as input parameters to the model.

So far, the model results agree with general trends of the metal deposition data, but further optimization of the model will be needed for better results. In the future, the developed model will be suitable for simulation of a wide range of HFB chemistries based on electrodeposition, further advancing the ability of energy storage producers to optimize flow battery (FB) systems.

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