Modelling PEMFC Degradation in Ships

Broer, A.; Polinder, H.; van Biert, L.

Publication date
2024

Document Version
Final published version

Citation (APA)
Broer, A., Polinder, H., & van Biert, L. (2024). *Modelling PEMFC Degradation in Ships*. 457-460. Paper presented at European PhD Hydrogen Conference, Ghent, Belgium.

Modelling PEMFC Degradation in Ships

A.E.Broer*[1], H. Polinder[1], L. Van Biert[1]

[1]Delft University of Technology — Department of Maritime and Transport Technology (MTT)

August 2023

Abstract

Switching to Proton Exchange Membrane Fuel Cell (PEMFC) systems can greatly reduce the environmental impact from the maritime industry. However, the limited durability of PEMFCs remains an obstacle for their implementation. Understanding fuel cell degradation is especially relevant for ships, as they typically operate for long periods and in isolated areas. Their energy systems therefore need to be exceptionally robust and reliable. In order to improve the design of maritime PEMFCs, we need to improve our understanding of degradation mechanisms induced by their use on a ship. Models can be a great tool to that end.

Many PEMFC models have been developed and used over three decades. They differ on various levels, from their spatial dimensions – one, two or three dimensional – to which processes are modelled and the detail to which they are described. Our previous review[1] shows that numerous processes contribute to degradation in a maritime context. These include more general processes, such as load induced damage, as well more specific ones for ships, such as sea salt contamination via the air inlet.

Currently, there is no modelling framework to quantify PEMFC degradation in a maritime environment specifically. The aim of this work is to propose such a framework, building on knowledge gained from previous modeling studies. It should integrate the additional degradation triggers such as salt contamination. We start out by analyzing existing PEMFC durability models. They are rated based on the coding complexity, computational costs, specificity and the possibility to incorporate both specific maritime as well as general degradation causes. Thereafter we analyze whether and how the models are validated and verified.

The proposed modeling framework can serve as a blueprint for future maritime PEMFC degradation models. These can facilitate vessel specific case studies, investigations to improve cell and stack design and explorations of altered ship operational profiles. The resulting insights will aid scientists, engineers and ship owners to improve PEMFC lifetime in maritime applications.

Introduction - Why do we need PEMFC degradation models for ships?

In a time of changing climate, fluctuating fossil fuel prices and ever growing international trade, innovations for sustainable shipping are urgently needed. Today, the maritime industry is responsible for about 3% of all anthropogenic greenhouse gas emissions worldwide, as well as 11% and 19% of all atmospheric sulfur and nitrogen oxide emissions within Europe [4, 3].

Hydrogen fuel cells (FCs) can greatly reduce the environmental impact of shipping as they have no polluting emissions. PEMFCs are amongst the most promising FCs types due to their ability to deal with fast fluctuating power demands, fast start-up, low operational temperature and high power density. Nevertheless, PEMFCs are also known for their limited lifetime compared to internal combustion engines and their sensitivity for contamination compared other fuel cell types. This is especially a risk as only few researchers have studied how the maritime environment will affect their performance and total lifetime.

Models have a great potential to advance PEMFC degradation research. Once developed, they can quickly provide results against low capital costs. These results can give insight in the working principles of fuel cells and the impact of operational conditions. It is therefore no surprise that many PEMFC models have been developed in the past decades, including ones that focus on degradation. However, to our knowledge, a dedicated maritime PEMFC degradation model has not been developed yet.

*Corresponding author: a.broer@tudelft.nl

[1]Review still under revision to be published. Abstract and conclusion are attached as the final page of this document.

Models vary widely in the applied approach and level detail. Spiegel et al ([7]) categorized the main model characteristics as: dimensions (zero to three dimensional); state (steady or dynamic); catalyst kinetics description; phases considered (liquid, gas or a mixture); mass transport description in the catalyst layer and membrane; inclusion of energy balances; and membrane swelling. On top of this, one can differentiate between empirical models that depend heavily on empirically obtained parameters and purely theoretical models. With this wide choice in models, it is challenging to select the effective and efficient approach.

Even if a suitable modeling approach is applied, models can still be worthless when they are not properly validated. Arif et al ([1]) pointed out that models can only be validated to a limited extent as various parameters cannot be independently measured in experiments. In addition the authors showed that most modeling studies only used one data set for model validation. Model verification is often not even mentioned in modeling studies. Nonetheless model verification is an important process to guarantee the correctness of model outcomes, even more when authors only have a limited amount of experimental data to initialize and validate the model.

The aim of this work is to propose a modelling framework for maritime PEMFC degradation simulations. It should conclude (i) which approach or approaches are most suitable for predicting performance decay caused by operation on a ship and (ii) a proper validation and verification plan. To reach this conclusion, we first define the model objective in more detail and provide a comprehensive overview of PEMFC degradation models. The latter are assessed on their coding complexity, computational costs, specificity and, most importantly, if they can be used to reach our main objective - maritime degradation modeling. Additionally, the validation and verification methods of each degradation model will be analyzed and compared to what is considered as 'sufficient' in dedicated validation and verification literature.

Background - PEMFC stack components and ensuring correct models

PEMFC components

Each PEMFC is composed of several layers as depicted in 1. The proton exchange membrane (PEM) is located in the center of the cell. Most PEMFCs use the commercial Nafion™, a perfluorosulfonic acid (PFSA) based membrane, for its adequate stability and good proton conductivity [2].

The membrane is flanked by an anodic and cathodic catalyst layer (CL). They are sometimes referred to as electrodes as the electrochemical reactions occur here. Each CL contains catalyst particles, a catalyst support and ionomer. Reactants and products are transported to and from the CLs via the pores in the gas diffusion layer (GDL), while freed electrons can exchange via its solid strands. Carbon based materials are often used, although metal based GDLs also occur.

The flow plates (i.e. current collectors) serve three main functions: conducting electrons to the external circuit, transporting reactants and products to and from the cell and providing structural support [5]. The layout of the flow-field can impact cell performance significantly. If the cell is part of a stack the flow plates are referred to as bipolar plates (BPs) as it has both an anodic and cathodic 'pole'. Finally, the cell is enclosed with two end plates (EPs), which compress the stack together and evenly distribute the pressure.

Most academic researchers test with single cells in order to save on capital costs and to limit confounding elements. However, in commercial applications these are stacked together in series. This way the overall potential difference increases, as does the output power.

Validation and verification

Model validation and verification are carried out to make sure the modeled outcomes are accurate and correct - at least, within the system boundaries for which it was designed. In model validation one checks if the outcomes are sufficiently accurate in comparison with an independent dataset of the modeled system. Aargent et al ([6]) summarize fourteen different validation techniques such as comparing modeled outcomes to outcomes of other, already validated models or using the model to predict the system behaviour.

Model verification concerns the correct implementation of code and overlap between the conceptual model and the computer model [6]. One should check if there are programming errors and if functions are implemented and initialized correctly. In general, more specialized and programming languages have a lower risk on programming mistakes.

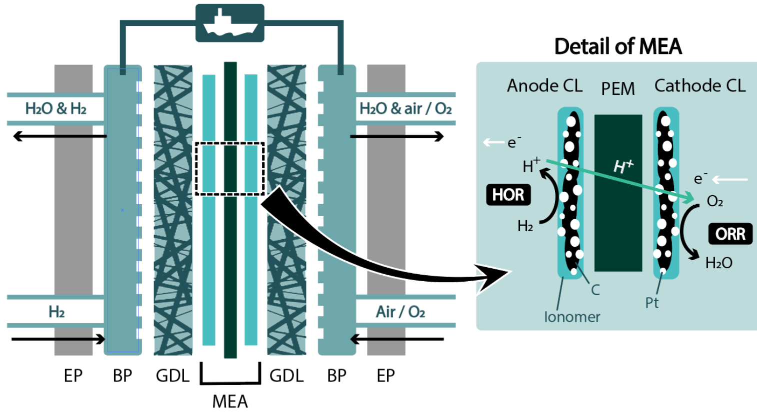

Figure 1: A schematic representation of a proton exchange membrane fuel cell (PEMFC). Its position in a stack (left) and a close up of the membrane electrode assembly (MEA, on the right) are indicated.

Methodology - Literature review, categorizing and framework outline

An initial set of literature will be collected via the Scopus search engine. Four search terms will be used: PEMFC, modeling, degradation and maritime. Maritime will be considered as an optional parameter, as we expect that there will be very few publications containing all four search terms. For each search term we try to improve our query by adding its synonyms, spelling variations and abbreviations. For example, the term PEMFC will be defined as *PEMFC, PEFC, "Proton exchange membrane fuel cell", "PEM fuel cell* or *"Polymer electrolyte fuel cell"* and modeling as *modeling, modelling, simulation, "theoretical model", "numerical model"* or *"computer model"*. The abstracts of the Scopus search results will be checked and relevant articles will be added to the literature list for this publication.

Discussion - code complexity, computational costs, specificity and maritime applicability

Expected outcome on types of PEMFC degradation models:

- Stack models or dedicated degradation models are scarce (most models focus on single PEMFCs or PEMFC components and aim to model performance at beginning of life (BoL))
- No dedicated maritime degradation models (most studies focus on automotive industry)

Expected outcome related to modeling approaches:

- Computational costs and model complexity go up with increasing dimensions and considering multiphase flows
- Model validation often occurs via comparison with one set of experimental data and only few describe the verification procedure

Conclusion - Most suitable modeling framework

Expected outcome:

- Two to three suitable model outlines for holistic modeling of maritime PEMFC stack degradation
- A validation and verification plan, using two sets of experimental data for validation and specific code checks for verification

References

[1] M. Arif, S. C. Cheung, and J. Andrews. Different Approaches Used for Modeling and Simulation of Polymer Electrolyte Membrane Fuel Cells: A Review. *Energy and Fuels*, 34(10):11897–11915, Oct. 2020. Number: 10 Publisher: American Chemical Society.

[2] A. Baroutaji, J. G. Carton, M. Sajjia, and A. G. Olabi. Materials in PEM Fuel Cells. In *Materials Science and Materials Engineering*. Elsevier, Jan. 2016.

[3] European Environment Agency. and European Maritime Safety Agency. *European maritime transport environmental report 2021.* Publications Office, LU, 2021.

[4] IMO. Fourth IMO Greenhouse Gas Study. Technical report, 2020.

[5] X. Li and I. Sabir. Review of bipolar plates in PEM fuel cells: Flow-field designs. *International Journal of Hydrogen Energy*, 30(4):359–371, 2005. Number: 4.

[6] R. G. Sargent. Verification and validation of simulation models - conference proceeding. Jan. 2011.

[7] C. Spiegel. *PEM fuel cell modeling and simulation using Matlab*. 2008.