Dataset Expansion and Normalization Refinement for GAF-CNN-Based Metal-Ion Concentration Prediction in Molten Salt

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***Keywords :** Cyclic Voltammetry, GAF image, Molten Salt, Data preprocessing, Machine Learning

1. Introduction

In high-temperature chloride molten salts, corrosion of structural materials can release metallic species such as Cr, Fe, and Ni into the salt, making continuous monitoring of dissolved metal ions important [1]. Cyclic voltammetry (CV) can be used to analyze the redox behavior of metal ions and to quantify their concentrations based on the current response [2].

In our previous study, CV data measured in a Static Cell were converted into Gramian Angular Field (GAF) images and analyzed using a CNN-based model for the classification and concentration prediction of five metal-ion species [3]. Although the model achieved a classification accuracy of 1.00, the overall coefficient of determination for concentration regression was only 0.567, indicating limited quantitative prediction performance. In addition, the previous dataset had limited coverage of concentration and experimental conditions, and the potential and current of each CV curve were independently normalized using their own minimum and maximum values, which could obscure absolute differences in signal amplitude.

In this study, the Static Cell CV dataset was expanded to five concentration levels of 0.10, 0.15, 0.20, 0.30, and 0.50 wt%. The normalization method was also revised by defining the potential range based on the Mg^{2+}/Mg and Cl_2/Cl^- reactions and applying a common fixed range to the current. The revised dataset and preprocessing method were then applied to the established GAF-CNN framework to reevaluate metal-ion classification and concentration prediction performance.

2. Experimental and Data Processing

2.1. CV Dataset Composition

In this study, the range of concentration and experimental conditions was expanded based on the Static Cell CV dataset used in the previous study [3]. The dataset consisted of five metal chlorides, $CrCl_2$, $FeCl_2$, $MnCl_2$, $MoCl_5$, and $NiCl_2$, in a 57:43 mol% NaCl-$MgCl_2$ mixture. The measurements were conducted at 773, 823, and 873 K with seven scan rates of 0.05, 0.10, 0.20, 0.30, 0.50, 0.80, and 1.00 V s^{-1}. Representative CV responses of the five metal chlorides are shown in Fig. 1.

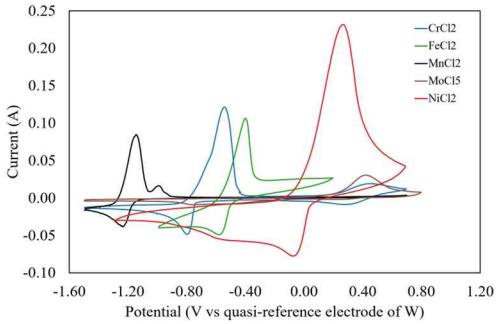


Fig. 1. Representative CV curves for five metal chlorides measured in the Static Cell.

In the previous study [3], a total of 108 raw CV data were used, with limited and uneven distributions of concentration and scan-rate conditions among the metal species. In the present study, the dataset was expanded to include five concentration levels of 0.10, 0.15, 0.20, 0.30, and 0.50 wt%. The final dataset consisted of 95 $CrCl_2$, 95 $FeCl_2$, 117 $MnCl_2$, 133 $MoCl_5$ and 104 $NiCl_2$ CV measurements, for a total of 544 CV measurements. The differences in the Static Cell dataset composition between the previous and present studies are summarized in Table I.

Table I: Comparison of the Static Cell CV datasets used in the previous and present studies

Item	Previous study [3]	Present study
Metal Chlorides	$CrCl_2$, $FeCl_2$, $MnCl_2$, $MoCl_5$, $NiCl_2$	$CrCl_2$, $FeCl_2$, $MnCl_2$, $MoCl_5$, $NiCl_2$
Temperature (K)	773, 823, 873	773, 823, 873
Scan rate (V s^{-1})	Species-dependent conditions	0.05, 0.1, 0.2, 0.3, 0.5, 0.8, 1.0
Concentration (wt%)	0.1, 0.3, 0.5	0.1, 0.15, 0.2, 0.3, 0.5
Number of raw CVs	108	544

2.2. CV Data Preprocessing and Normalization

In the previous study [3], the potential and current of each CV curve were independently normalized to a range from -1 to +1 using their respective minimum and maximum values. However, this approach may reduce differences in the actual signal ranges among different CV curves.

In this study, a common normalization criterion was applied to all Static Cell CV data. For potential, a common range from -1.6 V to +1.2 V was defined based on the Mg^{2+}/Mg reduction and Cl_2/Cl^- oxidation reactions observed in the blank NaCl–$MgCl_2$ CV, with the lower and upper limits mapped to -1 and +1, respectively. The potential range used for normalization is shown in Fig. 2. For current, a common range from -0.20 A to +0.20 A was mapped to -1 to +1. This approach enabled comparison of the relative signal magnitudes of individual CV curves using a consistent normalization basis rather than their individual minimum and maximum values.

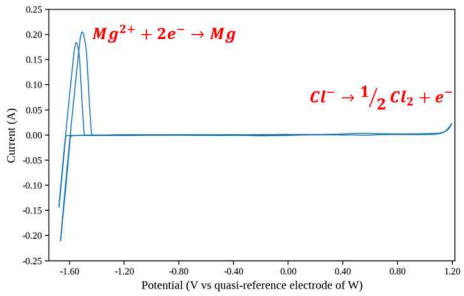


Fig. 2. Potential normalization range determined from the blank NaCl-$MgCl_2$ CV.

2.3. GAF Image Conversion and Model Evaluation

The normalized potential and current data were converted into Gramian Angular Field (GAF) images using the same method as in the previous study [3]. The GASF of potential was assigned to the red channel, the GADF of current to the green channel, and the GASF of current to the blue channel to construct RGB GAF images.

To examine differences in GAF representation according to the normalization method, GAF images generated using the previous per-CV min-max normalization and the revised fixed normalization were compared in Fig. 3. The entire dataset was divided into training and validation sets at a ratio of 80:20, with 109 CV measurements assigned to the validation set. The generated GAF images were used as inputs to the existing GAF-CNN model for metal-ion classification and concentration regression, and the performance was evaluated using accuracy and R^2.

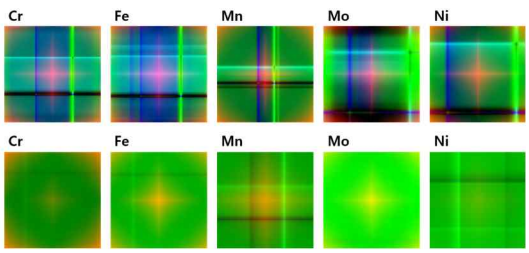


Fig. 3. Comparison of GAF images for five metal chlorides using the previous per-CV min–max normalization (upper row) and the revised fixed normalization (lower row).

3. Results and Discussion

The GAF-CNN model trained using the expanded dataset and revised normalization method maintained a classification accuracy of 1.00 for the five metal-ion species. The overall R^2 for concentration regression increased from 0.567 in the previous study [3] to 0.926 in the present study, and the species-specific R^2 values are summarized in Table II. In particular, the R^2 for $MnCl_2$ improved substantially from 0.156 to 0.869.

Table II: Comparison of concentration prediction performance between the previous and present studies

Metal Chloride	Previous study [3] R^2	Present study R^2
$CrCl_2$	-	0.940
$FeCl_2$	0.912	0.887
$MnCl_2$	0.156	0.869
$MoCl_5$	0.923	0.955
$NiCl_2$	-	0.953
Overall	0.567	0.926

The concentration predictions were assigned to nominal concentration levels of 0.10, 0.15, 0.20, 0.30, and 0.50 wt%, as shown in Fig. 4. Of the 109 validation samples, 88 were assigned to the corresponding concentration levels, while most mismatches occurred between adjacent concentration levels.

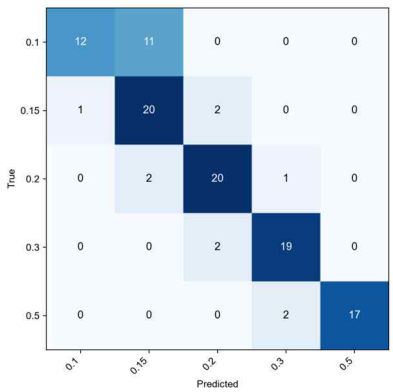


Fig. 4. Confusion matrix of predicted concentration levels for the validation dataset.

4. Conclusion

In this study, the Static Cell CV dataset was expanded, and the normalization method was revised to address the limited dataset coverage and per-CV normalization used in the previous GAF-CNN study. With the expanded dataset and revised preprocessing method, the model maintained a classification accuracy of 1.00 for the five metal-ion species, while the overall R^2 for concentration regression improved from 0.567 in the previous study to 0.926. These results demonstrate improved quantitative prediction performance of the GAF-CNN framework

with the revised dataset and preprocessing procedure. In future work, the model will be applied to MSTCL data to evaluate its prediction performance under flow-loop conditions.

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Acknowledgement

This work was supported by the Korea Institute of Energy Technology Evaluation and Planning (KETEP) and the Ministry of Climate, Energy & Environment (MCEE) of the Republic of Korea (No. RS-2023-00247323).
This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government (MSIT) (RS-2023-00261146).
This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education(RS-2025-25422439)