

Development of a Feature Extractor for a Concentration-Prediction Machine Learning Model Applicable to Molten Salt Environment

Yonadan Choi^a, Wonseok Yang^a, Sungyeol Choi^{b*}

^aDepartment of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology, 291, Daehak-ro, Yuseong-gu, Daejeon, 34141, Republic of Korea

^bSeoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul, 08826, Republic of Korea

*Corresponding author: choisys7@snu.ac.kr

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1. Introduction

As one of a type of Gen IV nuclear reactor, molten salt reactors use molten salt like chloride salt or fluoride salt as a core coolant. A molten salt reactor has many advantages compared to Gen III reactors. A molten salt reactor can be kept at the low-pressure condition, so it does not require thick pressure vessel to maintain the high-pressure condition like Gen III reactors. In addition, a molten salt reactor has higher passive safety since a molten salt is usually maintained in solid or liquid state and does not change its phase to gas during an accident, so large leakage of radioactive materials is prevented.

Despite its great advantages, there are some obstacles to be overcome until commercialization of a molten salt reactor. One of obstacles is the corrosion risk since molten salt is corrosive to structures of a reactor. The concentration monitoring of a corrosion products or corrosive products are important to analyze the current state and minimize the damage from corrosion. However, the direct online monitoring is limited as most commercial concentration sensors are not applicable to molten salt environments. Therefore, several indirect monitoring methods are required and suggested [1, 2].

As one of indirect monitoring method the electrochemical sensor let us know various information in a molten salt. To convert the measured data from electrochemical sensor into meaningful information it is important to extract essential features from measured data for machine learning. In this study, the development of a feature extractor for machine learning is presented. The developed feature extractor could be used to develop the machine learning model and the online monitoring system for molten salt reactors.

2. Methods and Results

There are several types of electrochemical measurement methods. Cyclic voltammetry, chronoamperometry and linear sweep voltammetry are examples of electrochemical measurement methods. In this section, the selected features and the methods to extract those features are introduced. The feature extractor is developed with Python since Python provides easy and meaningful libraries for data processing.

2.1 Cyclic Voltammetry Extractor

Cyclic voltammetry is the method that increases and decreases voltage in the specific range and observes the current trend at the electrode. Berzins-Delahay equation shows the relation between a concentration and a peak current in voltage-current curve [3, 4].

$$I_p = 0.61AC_i\sqrt{\frac{F^3n^3D_i\nu}{RT}} \quad (1)$$

(I_p : Peak current, A : Electrode surface area, C_i : Concentration of the nuclide i , F : Faraday constant, n : Number of electrons that participates in reaction, D_i : Diffusion coefficient of nuclide i , ν : Voltage scan rate, R : Ideal gas constant, T : Temperature)

As it can be inferred from equation 1, the electrode surface area, peak current, and some other variables are related to the concentration of a nuclide. In addition, the previous study suggests that the area of the voltage-current curve has relation with the concentration of a nuclide [5]. Therefore, it is designed to extract the below features from cyclic voltammetry data.

- 1) Peak potential/current (Reduction/Oxidation)
- 2) Whole Area
- 3) Peak Area (Reduction/Oxidation)

To find a peak potential and current, the data is smoothed by averaging data of 5 indices successively. The `find_peaks` function in `scipy.signal` library is used to find peaks. However, the `scipy.signal` library is usually used in signal processing field where the base signal is flat and definite peaks exist in the signal. On the contrary, the base of voltage-current curve is not flat (the current value is different before and after the peak appears). Accordingly, the hyperparameters of the `find_peaks` function is adjusted to find the peak optimally.

Figure 1~4 shows the examples of observed peak current, whole area calculating range, peak area calculating range, and the capacitive current considered peak current, respectively. Peak candidates are expressed with translucent green diamond. Among them, finally

extracted peaks are expressed with blue squares for reduction peaks, and red squares for oxidation peaks.

Both whole area and half area are calculated with trapezoidal method. However, potential points of reduction and oxidation do not match each other, so area of reduction and oxidation region is calculated separately. To calculate half area, the point found by find_peaks function with 0.5 of rel_height is used. This way, the half position of the peak can be known.

Lastly, the feature extractor provides the option whether to consider capacitive current or not. The capacitive current is the base current which is not concerned with the reaction that produces peak. The capacitive current can be calculated by drawing tangent line at the region before the peak occurs (Fig 4).

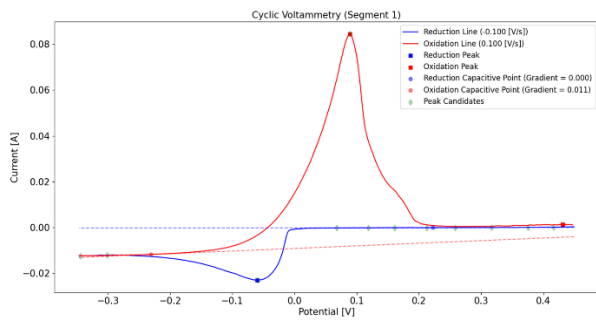


Fig. 1. Observed Peak Current in Voltage-Current Curve

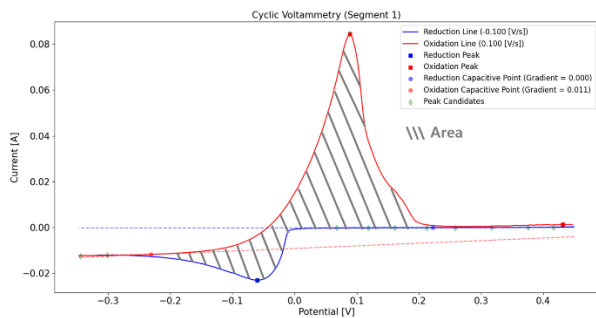


Fig. 2. Whole Area in Voltage-Current Curve

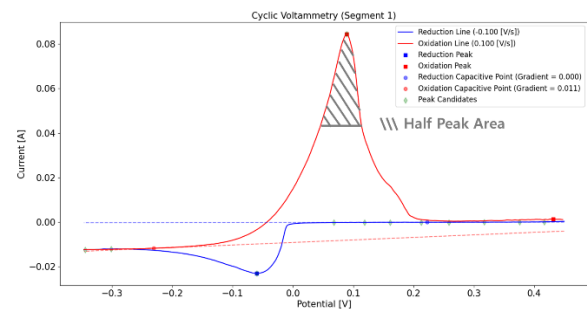


Fig. 3. Peak Area in Voltage-Current Curve

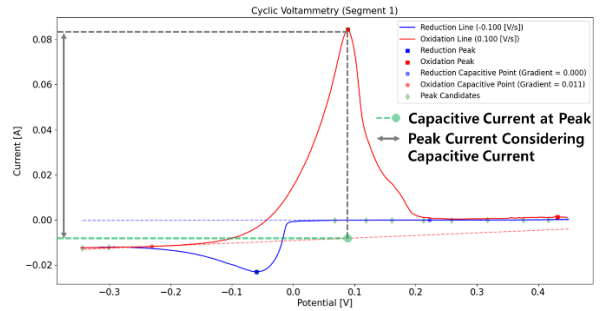


Fig. 4. Considering Capacitive Current in Voltage-Current Curve

2.2 Anodic Stripping Analysis (Chronoamperometry & Linear Sweep Voltammery)

Anodic stripping analysis consists of the deposition step (Chronoamperometry) and the stripping step (Linear Sweep Voltammery). During the deposition step, the deposited charge, initial deposition current and final deposition current could have relation with the concentration of a nuclide. On the other hand, during the stripping step which is also called as linear sweep voltammery is the half of the cyclic voltammery. The voltage is increased from the voltage value applied at deposition step to the end voltage value set. Thus, the same features which are extracted from the cyclic voltammery are extracted during the stripping step (Peak potential/current, Whole area, half peak area).

2.3 Extracted Features and Analysis

The example of extracted data is like figure 5. In column B, salts used in experiments are shown. SME is the abbreviation for Sodium chloride with Magnesium chloride. In column C, nuclides used in experiments are shown. In this study, the feature extractor is used for experiments which include FeCl_2 and CrCl_3 or CrCl_2 . Column D shows the temperature of the experiment.

Column F and G shows the electrode information. As two electrodes where one is long and the other is short are used, the inserted length of short electrode and the length difference between the long and the short electrode is shown in column F and G, respectively.

From the column H, features which are mentioned at previous sections are shown. Features from the long electrode is expressed with letter "L" and features from the short electrode is expressed with letter "S" between parentheses. In addition, scan rates or deposition potentials are expressed after the electrode long/short index. Lastly, the reduction or oxidation is distinguished by letter "R" and letter "O" in some columns where both reactions need to be distinguished.

Fig. 5. Extracted Data File Example

Using these extracted features, correlation coefficients are investigated between area ratio and some features, and between concentration and some features. Figure 6 shows the correlation heatmap between area ratio and each peak current ratio in various conditions. Figure 7 shows the correlation heatmap between concentration and each peak current flux in various conditions.

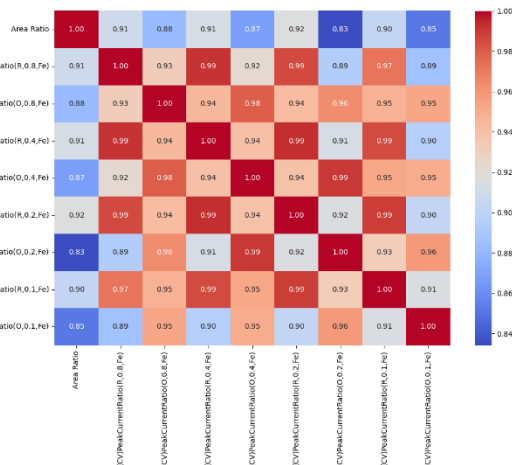


Fig. 6. Correlation Heatmap between Area Ratio and Peak Current Ratios

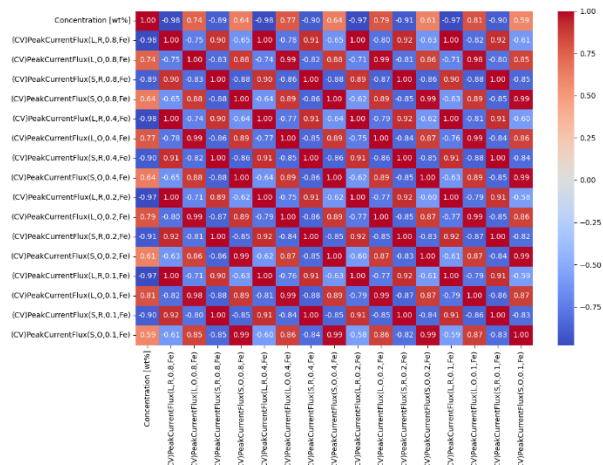


Fig. 7. Correlation Heatmap between Concentration and Peak Current Flux

It could be observed that all peak current ratios show correlation coefficients higher than 0.8 with area ratio, which is one logistic conclusion. Additionally, reduction

peak current ratios show higher correlation coefficients than oxidation peak current ratios. This may be caused by the influence difference of capacitive currents in the reduction and oxidation. Reduction peaks are not affected by capacitive currents as a extended line of capacitive current is almost flat, whereas oxidation peaks are affected more than reduction peaks.

Similarly, the reduction peak current flux showed higher correlation coefficients compared to the oxidation peak current flux. Furthermore, it is observed that the peak current flux from the long electrode has higher correlation with the concentration than the short electrode, which is another logistic conclusion. As logistic conclusions are derived from the correlation heatmap between features, it could be concluded that the feature extractor extracted peak current features with a small error.

3. Conclusions

The feature extractor for a concentration-prediction machine learning model is developed in this study. This feature extractor can act as a data preprocessor for machine learning of a concentration prediction model applicable to molten salt environment. Additionally, if this feature extractor is connected to the electrochemical sensor and trained concentration prediction model, that combination can act as a real-time virtual concentration sensor.

The developed feature extractor can extract the essential features from several electrochemical measurement methods such as cyclic voltammetry, chronoamperometry and linear sweep voltammetry. From the correlation heatmap between area ratio and peak current ratios and between concentration and peak current flux, logistic conclusions are well derived. Accordingly, it is concluded that the feature extractor extracted peak current features with a small error.

However, features from anodic stripping analysis (Chronoamperometry and linear sweep voltammetry) are not analyzed primarily in this study since they showed poor quality to be used in concentration-prediction machine learning model. Therefore, the next step for the development of the feature extractor would be finding the meaningful features from other electrochemical measurement methods except the cyclic voltammetry and developing extracting function of those features. In addition, it should go through more verification process with various experiment data for its versatile application.

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