

An Open Access Code to help you Estimate Transport and Kinetic Parameters of Vanadium Redox Batch Cell Systems

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There are two sets of source codes, executable files, and text files for the Nafion[®] 115 and the Nafion[®] XL systems. They are prepared to run on any Windows based PC environment. Each set contains a source code, an executable file, and five text files. All relevant files can be downloaded directly from Dr. Seongbeom Lee's website as a zip file (www.seongbeomlee.com). Download [here](#) for the the Nafion[®] 115 system and [here](#) for the Nafion[®] XL system. Once the zip files are downloaded, unzip all the files into the same folder. Below is the detailed instruction.

The Nafion[®] 115 system. The executable file ('Estimation_Nafion[®] 115 system.exe') in the zip file can estimate five parameters of the Nafion[®] 115 system: rate constants at anode and cathode, the cell resistance excluding the membrane resistance, the diffusion coefficient of protons, and the formal potential. The executable file uses one set of CC-CV charging and one set of CC discharging profiles and text files for specifying the experimental and model conditions.

1. Experimental conditions: While specifying the experimental conditions, information such as (i) the value of applied current, (ii) the regular time interval for a profile, and (iii) the number of voltage data used for parameter estimation exercise etc. are required. Users can enter their own experimental conditions to the text file called "Experimental conditions.txt". For the parameter estimation exercise carried out here, the following information has been entered. The first row is provided to enter values of applied currents for CC-charging and CC discharging for Nafion[®] 115 system at one C-rate. The provide text file contains values such as 0.000893 (C/30) for the first row. The second and third rows represent time intervals of CC-charging and CC-discharging at C/30 rate. In the uploaded text file, these time intervals were set as 513.67 and 362.46 seconds for the C/30 operation. In the last row, users need to enter the number of the experimental data used for parameter estimation exercise. In this case, this number has been entered as 200.
2. Voltage data: Provide experimental voltage data at your C-rate (e.g., C/30) in the file called "Voltage data.txt". Note that the same number of experimental data was prepared for charging and discharging profiles. The first row represents the number of experimental data. The second and third columns present voltage data for charging and discharging at C/30, respectively. Users can input their experimental data sequentially.
3. Bounds: Provide bounds for estimating parameters in the "Bounds.txt" file. The first row represents the total number of bounds. After that, the lower and upper bounds for each of the five estimating parameters are given in this file as an 5 rows by 2 columns array. The parameter bounds are given in the following sequence: rate constants at anode and cathode, the formal potential, the diffusion coefficient of protons, and the cell resistance excluding the membrane resistance.
4. Initial guess: Provide initial guesses for estimating parameters in the "Guess.txt" file. Five estimating parameters are given in this file as a 5 rows by 1 column array. The initial guesses are given in the following sequence: reference rate constants at anode and cathode, the formal potential, the diffusion coefficient of protons, and the cell resistance

excluding the membrane resistance. This sequence is same as the above sequence for providing the bounds for the parameters.

5. Model condition: Provide mathematical conditions such as the number of Ordinary Differential Equations (ODEs) and Algebraic Equations (AE) and tolerance in the text file called “daskrinput.txt”. The number of ODE, the number of AE, a relative tolerance, and absolute tolerance are presented sequentially.
6. Double click and run the execution file “Estimation_Nafion® 115 system.exe”. Upon clicking, a command line window will be opened, and the program will calculate the optimal values of parameters. Once finishing the calculation, the command window will be closed. No action required.
7. The optimization results for all the variables can be found in the “Estimated parameters.csv”. The results will be given by the following sequence: rate constants at anode and cathode, the formal potential, the diffusion coefficient of protons, and the cell resistance excluding the membrane.

The Nafion® XL system. The second program (“Other membrane system.exe”) can estimate diffusion coefficients of four vanadium ions and protons for other membranes. The protocol to execute the executable file is similar to the previous step.

1. Identify your experimental conditions. Users can enter their own experimental conditions in the “Experimental conditions.txt” file. In the uploaded text file, the first row represents a value of applied currents for CC-charging for the Nafion® XL system at C/30. The second and third rows represent time intervals of CC-charging and CC-discharging. Here, the time interval was entered as 446.7550251 and 105.1483133 seconds for charging and discharging at C/30. In the fourth row, users need to enter the number of the experimental data. In the original file, the number of 200 experimental voltage data was used. From the fifth to the seventh rows, the information obtained in the Nafion® 115 system was used i.e. the fifth and sixth rows represent rate constants at anode and cathode, the seventh row represents the cell resistance, and the formal potential.
2. Bounds for estimating parameters are entered in the “Bounds.txt” file. The total number of bounds is given in the first row. After that, the bounds are given as a 5 rows by 2 columns array, i.e. the lower and upper bounds are given for the estimating parameters in the following sequence: diffusion coefficients of V^{2+} , V^{3+} , VO^{2+} , VO_2^+ , and protons.
3. Voltage data: Provide experimental voltage data at one C-rate in the file called “Voltage data.txt”. Note that the same number of experimental data was prepared for charging and discharging profiles. The total number of experimental data is given in the first row. After that, the first and second columns present voltage data for charging and discharging at C/30, respectively. Users can input their experimental data sequentially.
4. Initial guess and model conditions: Provide initial guesses for estimating parameters into the “Guess.txt” file. Five estimating parameters are given in this file as a 5 rows by 1 column array. The initial guesses are given in the following sequence: diffusion coefficients of V^{2+} , V^{3+} , VO^{2+} , and VO_2^+ , and protons. Also, provide mathematical conditions including the number of ODE and AE and tolerance. The text file called “daskrinput.txt” includes the number of ODE, the number of AE, a relative tolerance, and absolute tolerance sequentially.

5. Double click and run the executable file “Other membrane systems.exe”. Upon clicking, a command line window is opened, and the program will calculate the optimal values of the parameters. Once finishing the calculation, the command window will be closed. No action required.
6. The optimization results for all the parameters can be found in the “Estimated parameters.csv”. The results will be given by the following sequence: diffusion coefficients of V^{2+} , V^{3+} , VO^{2+} , and VO_2^+ , and protons.

*Code released with restrictions. Free for academic use but not for commercial purposes.

*For details on restrictions please contact sblee3487@gmail.com