DELIVERABLE REPORT

Deliverable no. / title:	D3.8 KMC software deposite in GitHub
Lead beneficiary:	CNRS-LRCS
Nature of deliverable:	Report
Dissemination level:	PU– Public
Due date:	M36 / December 2022
Grant Agreement number:	875489
Project acronym:	SONAR
Project title:	Modelling for the search for new active materials for redox flow batteries
Funding scheme:	H2020-LC-BAT-2019
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Project website:	www.sonar-redox.eu
Project website:	This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement no. 875489. This report reflects only the authors' view. The funding agency is not responsible for any use made of the information it contains.

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1 Introduction

This delieverable describes the kinetic Monte Carlo software developed in WP3 for Task 3.1, Task 3.3 and Task 3.4.[1] The software is uploaded to the GitHub in the following repositories (Figure 1.):

https://github.com/Jessy-YU-Aws/SONAR_Delieverable3.8

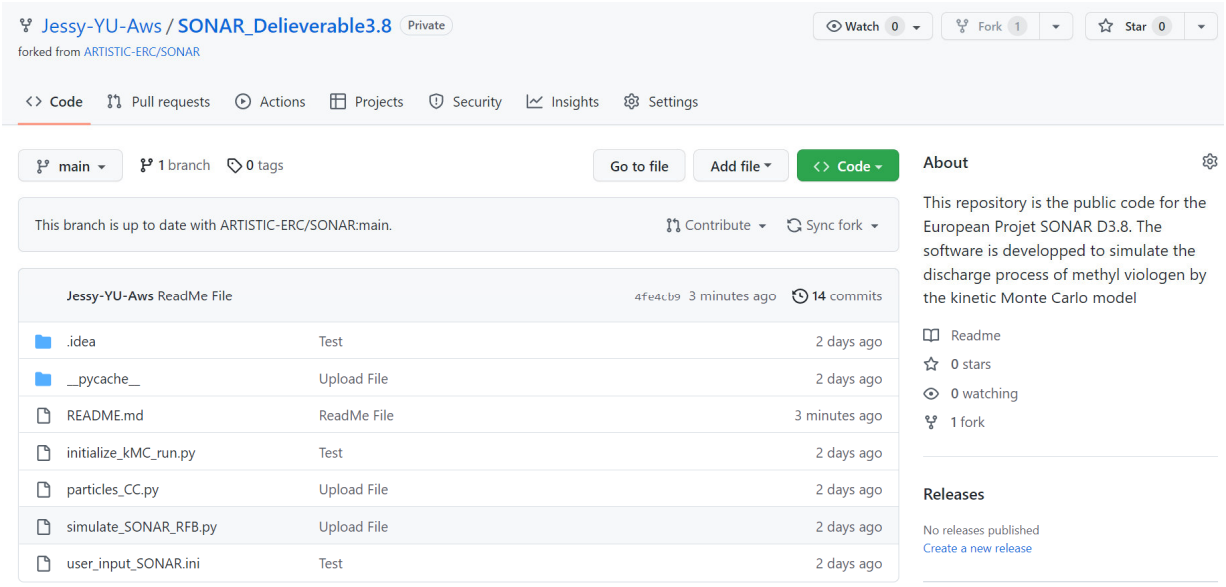

Figure 1. Screenshot of the Github repository.

2 KMC model for users

This python coded model aims to simulate the discharge of the anode materials in a redox flow battery system. The defaut material is methyl viologen. The discharging process is simulated by kinetic Monte Carlo algorithm. In each iteration, the algorithm chooses one event to execute and update the system configuration.

The main function is written in the 'simulate_SONAR_RFB.py'. The related kinetic Monte Carlo algorithm is coded in the 'particles_CC.py'. The 'initialize_kMC_run.py' is for initialization the input parameters. The input parameters can be altered in 'user_input_SONAR.ini'

There will be three output files. The output file with '.txt' records the simulation results, including the simualtion time, time step, electrode charge density, the potential drop thorugh the compact layer, the potential on the interface between the compact layer and the diffuse layer, and the type of events. The output file with '.xyz' records the location of each ions. To visualise the 3D configuration of the simualtion box, users can use the software Ovito to process. The output file with '.log' is the logfile which doesn't contain simulation results.

To launch a simulation, users need to type the following line in the terminal : 'python simulate_SONAR_RFB.py'

3 Next steps

Different branches will be added to the repository, including the post-processing code, the kMC based mean square displacement model developed in Task 3.5, and another Butler-Volmer equation combined with kMC model.

4 References

1. Yu, J., Shukla, G., Fornari, R.P., Arcelus, O., Shodiev, A., Silva, P. De, and Franco, A.A. (2022) Gaining Insight into the Electrochemical Interface Dynamics in an Organic Redox Flow Battery with a Kinetic Monte Carlo Approach. **2107720**, 1–13.