

LLNL-SCDC (LLNL Surface Complexation Database Converter)

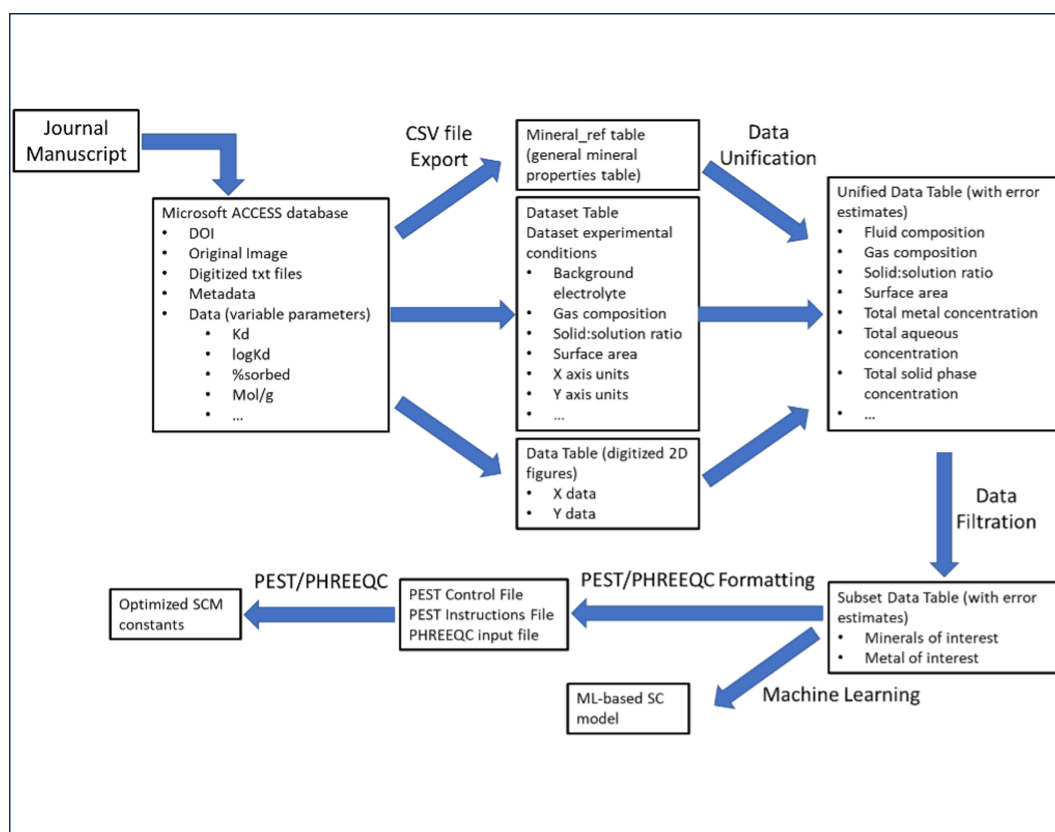
Category
Software

SCDC is a R-based script that creates a unified dataset of surface complexation experimental data with respective parameters and results

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Description

The Lawrence Livermore National Laboratory Surface Complexation Database Converter (SCDC) is a R-based script that creates a unified dataset of surface complexation experimental data with respective parameters and results. To provide context, it is commonly understood in the data science community that gathering and cleansing data can take up to 80% of the time in analytics - with the remaining 20% being the actual analysis. This script turns the 80% process of data cleansing into a more seamless, time efficient process. The LLNL SCDC consists of three process tabs: (1) Unifier, which reads a Dataset/Data .csv and a mineral reference Excel file in order to create a collective dataset, (2) Filterer, which reads in the output from the Unifier to filter for specific mineral-sorbent pairs, and (3) Formatter, which reads the output from the Filterer to prepare the dataset for future data manipulation and processing. The server.R, ui.R scripts, and all necessary Excel/.csv files for running the SCDC are presented in this public release to allow for scientists to more easily compile experimental data on metal-mineral surface interactions.



References

1. Zavarin, M.; Chang, E.; Wainwright, H.; Parham, N.; Kaukuntla, R.; Zouabe, J.; Deinhart, A.; Genetti, V.; Shipman, S.; Bok, F.; Brendler, V.(February 1, 2022) ,
<https://pubs.acs.org/doi/10.1021/acs.est.1c07109>, Environmental Science & Technology, 56(4), 2827-2838