**Main Scripts:**

CurveFitting\_V13\_Optimization.m: Run this script first when analyzing new data. This script pulls the experimental data, and the experimental diffusion coefficients, and finds the optimal parameters to fit the diffusion model to each physical experiment. The outputs are then to the Results/Minimums folder. This script takes quite some time to run for all 46 experiments, as we optimize starting from multiple different seeding points in the parameter space, for three different possible diffusion coefficients.

CurveFitting\_V13\_Visualization.m: Run this script after CurveFitting\_V13\_Optimization. This script takes the diffusion model parameters generated in the optimization run and calculates the final concentration profiles and visualization for each experiment. The various results are saved in the Results folder.

**Functions:**

DiffusionAllSpeciesV2.m: This is the mathematical model for diffusion and is run in the backend each time the main script simulates an experiment.

DiffusionAllSpeciesV2Visualization.m: Same as DiffusionAllSpeciesV2.m, with some edits to output visualizations.

DiffusionSSE3.m: This is the objective function that is called in CurveFitting\_V13\_Optimization.

LinearInterp.m: This is used to linearly interpolate concentration values between the centers of each of the discrete bins.

LinearInterpV2.m: Based off LinearInterp, this is used in CurveFitting\_V13\_Visualization for generating the final graphics.

StartingCalculationsV3.m: Calculates the starting moles, heights, and concentrations of the species given the experimental data.

StartingCalculationsV2.m: Calculates the starting moles, heights, and concentrations of the species given the experimental data. This calculates fewer species than StartingCalculationsV3, and is still used for some preliminary checks.

binmergeV1.m: Used in DiffusionAllSpeciesV2 to merge bins together once they get too small.

binspawnv2.m: Used in DiffusionAllSpeciesV2 to split bins once they get too large.

diffcalcV1.m: The finite difference calculation used by DiffusionAllSpeciesV2.

**Required Data to Run:**

Diffusion\_Coefficient\_Data.csv: This spreadsheet provides the experimental diffusion coefficients.

Google Spreadsheet:

https://docs.google.com/spreadsheets/d/1D\_4OouMg8elj\_djLPVKltK7Yq\_Urgayx4KI2zEomAEE/edit#gid=0