Here I am using CO2 as an example to show how to generate the training dataset for CO2 and using the calibration code to generate new model for alpha. The use that to predict the CO2 density values.

1. Go to Equation of state research,WEI/data & tecplot/carbon dioxide, click excel file CO2 density.xlsx, then copy the density values and their corresponding pressure values in the excel file.
2. Open the Matlab code, CO2\_sat\_alpha.m. Drag the excel file into the command window. Then a new window will pop out. Set the output style as column vectors. Select the density values and their corresponding pressure values you just put in the excel file, import the data into your Matlab workspace.
3. Create a new script in Matlab. Put in the code, save document\_name.mat (here I used, save CO2\_sat\_data1.mat) and run it in the same environment. You will see a new file document\_name.mat has been created in the file.
4. After that, Run the code CO2\_sat\_alpha.m . Make sure you change the 3rd line load CO2\_sat\_data1.mat to the same file name as you used for the ‘save ‘command. If you want to use a different temperature, you need to change the initial temperature line 22, the looping number line 27 and the increasement of the temperature line 44.
5. Then the values of the variable ‘alpha\_PR\_liq’are the training alpha values.
6. You can save the training alpha values in the excel file CO2\_sat\_alpha.xlsx.
7. Then go to Equation of state research,WEI/calibration no noise/carbon dioxide
8. Open the R code, calibration\_no\_noise.R
9. Set the working path as Equation of state research,WEI/calibration no noise/carbon dioxide
10. Put the new training dataset (including Tr, Pr and alpha) in raw alpha for exp\_data.csv and alpha.csv
11. Run the code
12. The prediction results (including the new alpha values) will be saved in predictions.csv
13. Then use the MATLAB code carbon\_dioxide\_density\_pridection\_220\_800.m to get the density value1
14. Save the new alpha values in CO2\_alpha.mat(the save way as mentioned before), then you may need to change the code, line 16(depends on how many different pressures), line 17(initial temperature), line 14(pressures), line 18(how many temperature values), line 15
15. Then run the code, the liquid and vapor density values will show up in the working area, you can use the excel file CO2 T rho1.xlsx to collect the density values.