The goal of this study is to use different sensor types to be able to use their characteristic responses from different gasses to predict individual ones that could occur in a mixture. In this case, we used natural gas (70% methane) and gasoline vapors and introduced them into a sensor array that was populated with a combination of Figaro metal oxide sensors, E2V metal oxide sensors, and a Baseline Mocon Photo-ionization detector. The mixing ratios ranged from 0 (zero air) to ~ 4 ppm gasoline (total VOC), 0 to ~120 ppm CH_4. Note that in all the plots below, methane has been divided by 10 so that they can be shown in the plots at similar magnitudes to those of gasoline. The apparatus is set up to perform a third gas (in this case CO) but in this case, only two components were used for simplicity and CO was kept at zero. Figure 1 shows the mixing ratios or gasoline and CH_4 as a function of time. In the first 1/3 of the tests, gasoline was ramped from zero to ~ 3 ppm in 8 steps. Next, gasoline was turned off and CH4 was ramped up. Then, the mixture of the two gasses were introduced into the mixing/measurement chamber in a variety of ratios. The total number of "tests" was 21. Next, a 2nd set of experiments were performed where the original gasses were introduced into the chamber with ± 10% variation in the individual flow rates as in the first case. The reason for this second case was to provide a different (but similar) "experimental" set to determine if the training results of the first test could accurately predict the concentrations of the 2nd test based on the sensor responses. The original mixing ratios ("training set") are shown in the top panel and the 2nd set of tests ("prediction") are shown in the bottom panel of Figure 1.

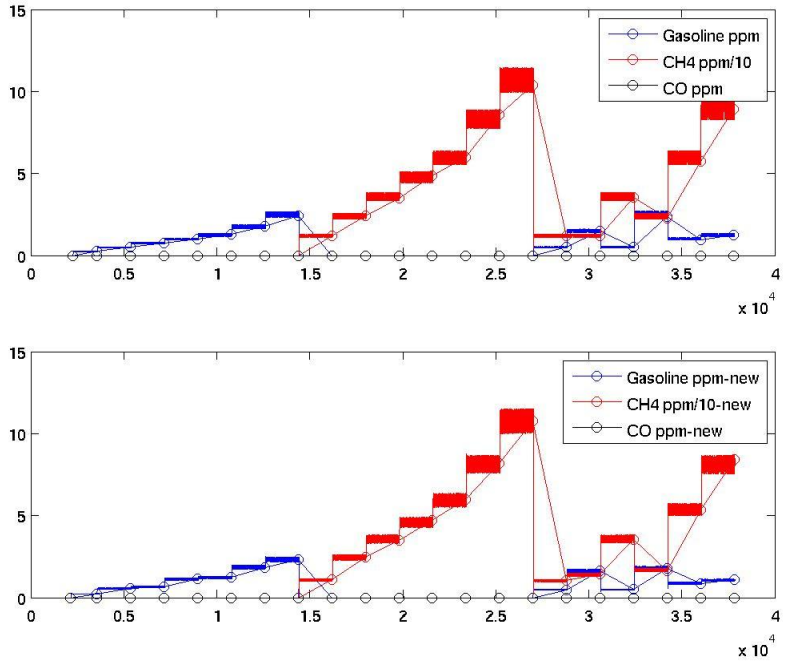


Figure 1: Mixing ratios of gasoline vapors and CH4/10 vs. time for original (top) and modified data set (bottom).

Figures 2 and 3 shows the results of the sensor responses based on the mixing ratios shown in Figure 1. There were two types of Figaro VOC sensors used (2600 and 2602) and one type of e2v sensor (5121). Although not used in this particular example, a CO sensor (e2v model 5525) was used, and for completeness, the response from this sensor are also shown.

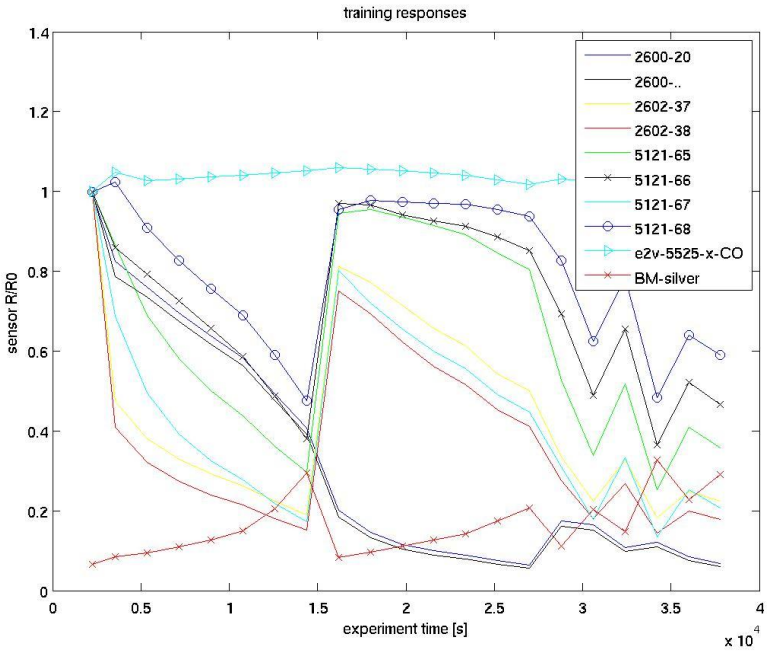


Figure 2: Sensor responses for mixing ratios of first tests shown in the top of Figure 1.

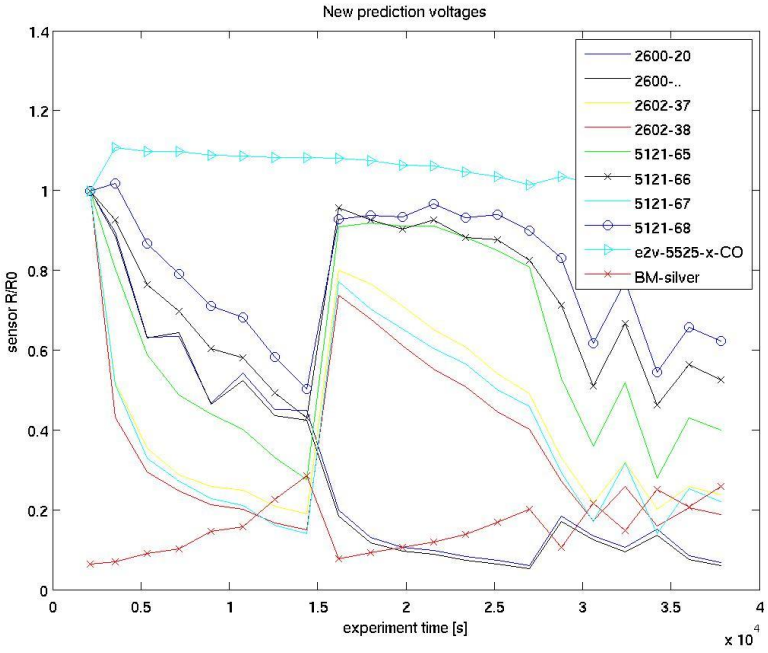


Figure 3: Sensor responses for mixing ratios of 2nd test shown in the bottom of Figure 1.

The neural networks technique was used to predict the responses of the secondary data set based on the relationships ("training" set) determined from the sensor responses used above. 4 sensors were used as the inputs to the neural network model:

1. One Figaro 2600 VOC
2. One Figaro 2602 VOC sensor
3. One e2v 5121 VOC sensor
4. One Baseline Mocon PID sensor for VOC

The predicted variables (2 concentrations) were the mixing ratios of CH4 and gasoline. The predictions were used to estimate the concentrations of the two gasses (shown in the bottom of Figure 1) based on the sensor responses in the 2nd test shown in Figure 3. Figure 4 shows the results of these predictions. Note that the first 1/3 of the tests were zero air followed by gasoline only ($CH_4 = 0$), the 2nd 1/3 of the tests had increasing CH_4 (gasoline = 0) and the last third had mixture of the two gasses.

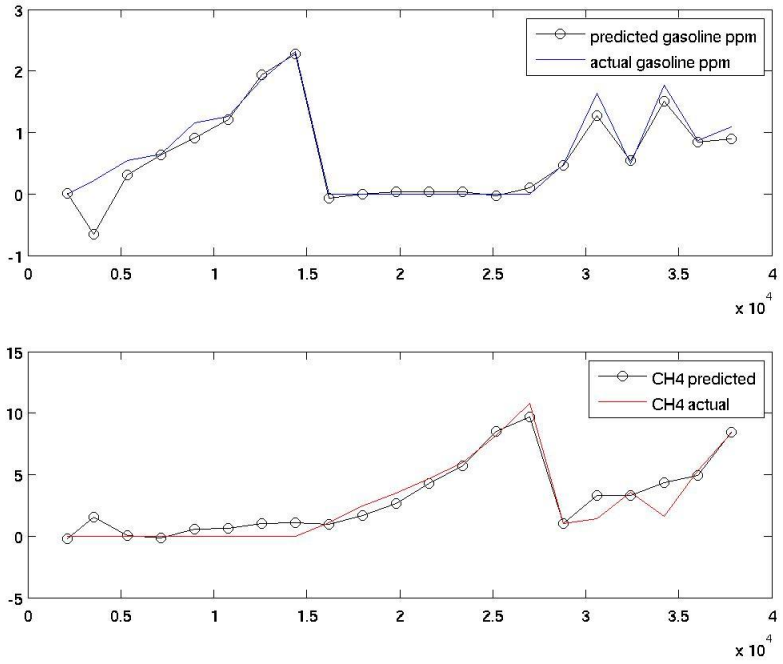


Figure 4: Actual and predicted CH_4 and gasoline mixing ratios. Solid lines indicate actual concentrations, while lines with open circles indicate predicted values.

Figure 5 shows the point-wise correlation between the predicted concentrations and the actual concentrations from Figure 4. Figure 6 shows the difference between actual and predicted concentrations. The fit is encouraging, as the delta is close to zero for all time periods. The fit for gasoline is better than it is for methane. More work is underway to do more random and/or continuous concentration changes of these two gasses alone and with CO to determine the robustness of this technique.

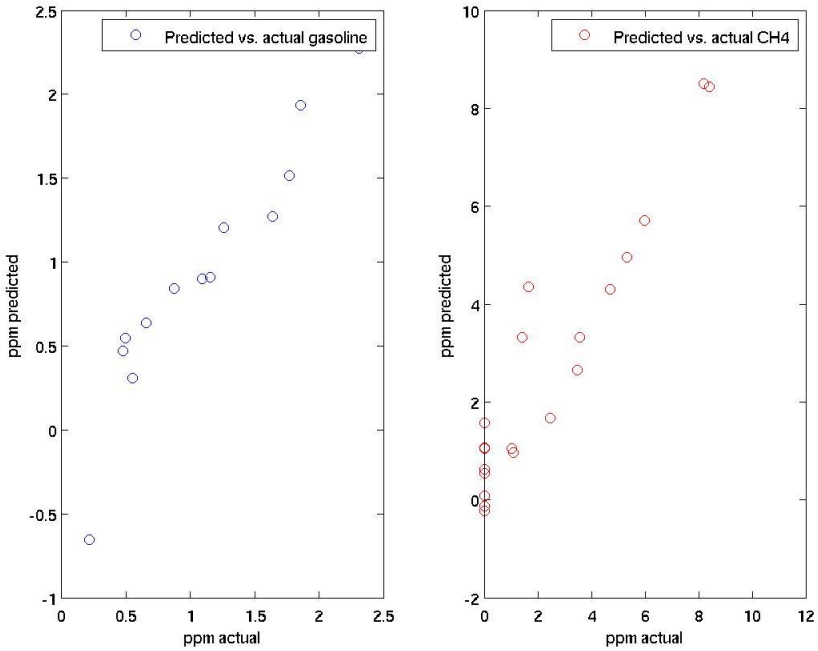


Figure 5: Predicted vs. actual concentrations for gasoline (left) and methane (right).

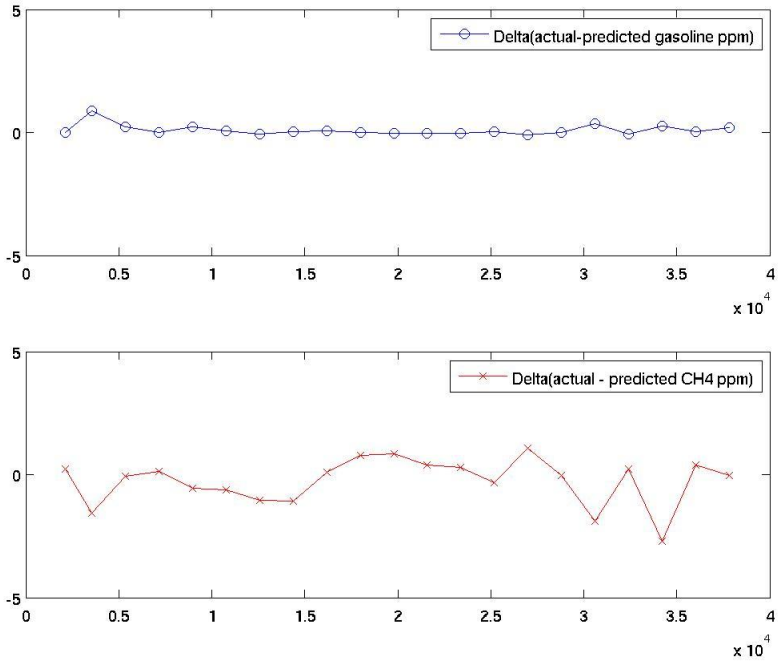
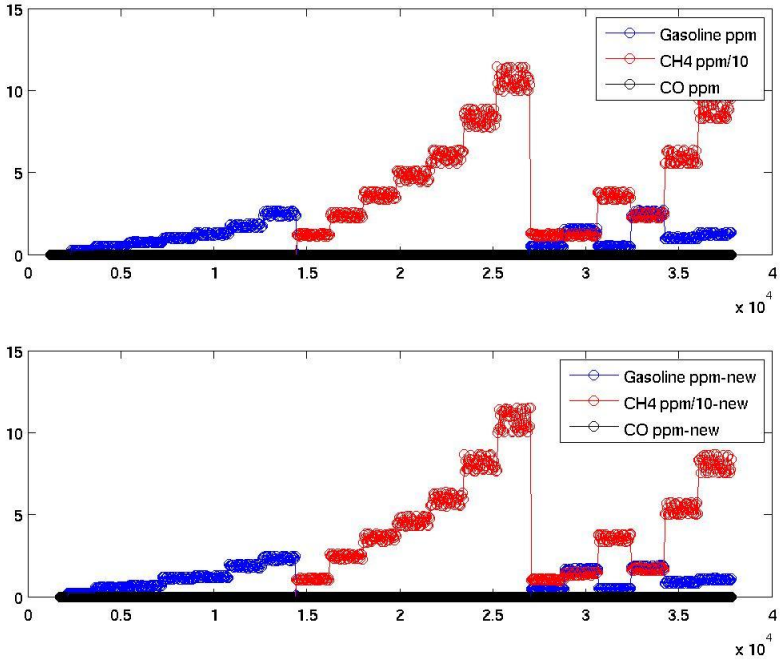
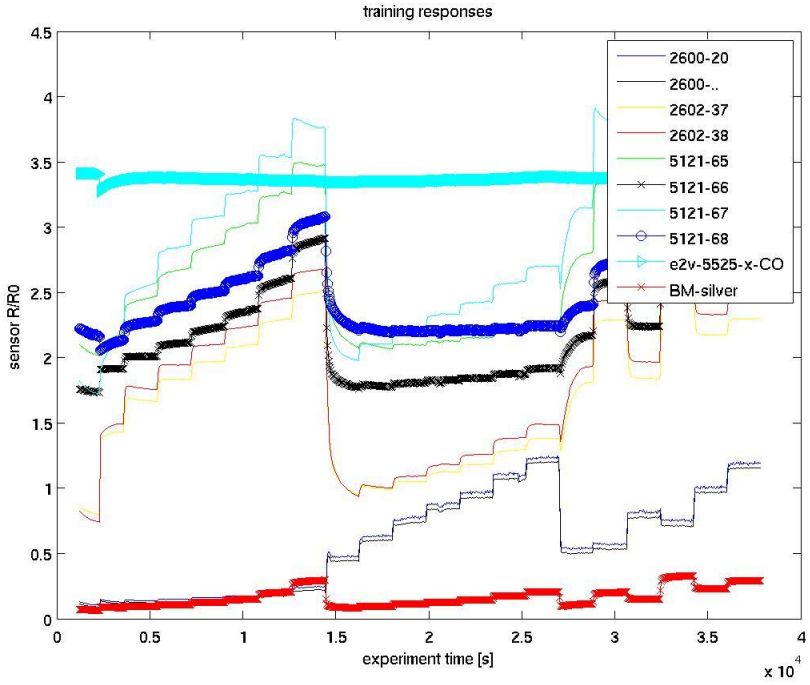


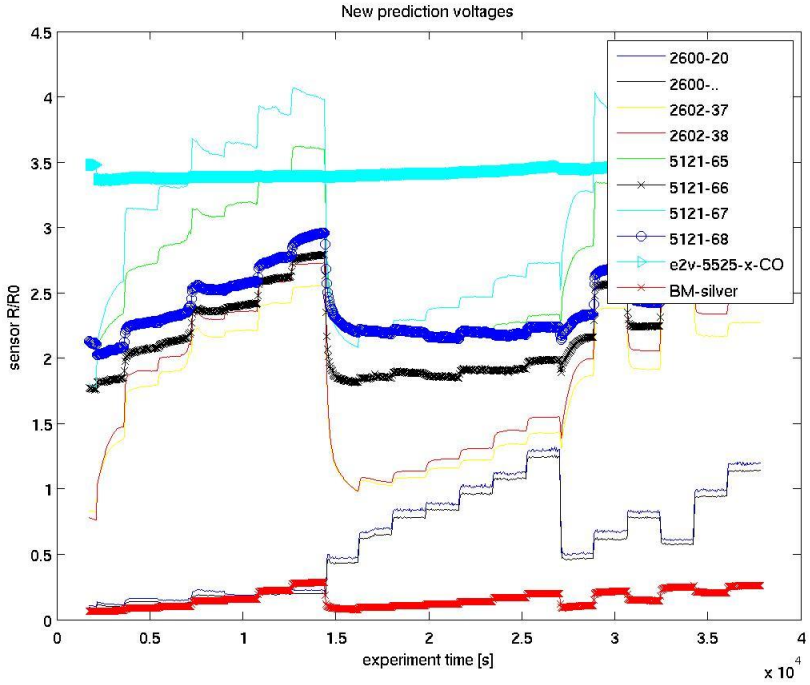
Figure 6: Differences between actual concentrations and predicted concentrations for gasoline (top) and CH_4 (bottom).

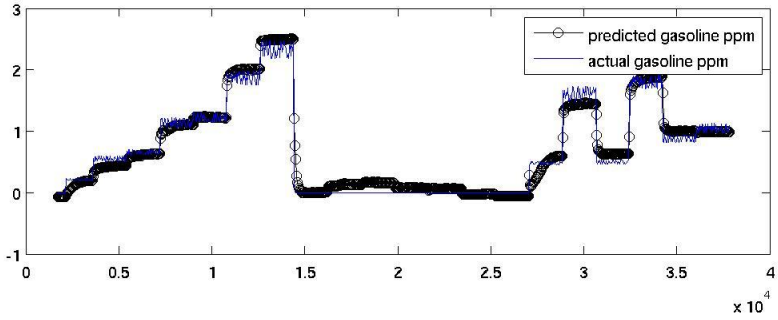
The neural network analysis above was performed with just the steady state responses at each step. The analysis was also performed with more data points (using every 20^{th} data point) and the corresponding figures (to 1-6) are shown below. In this simple case, the

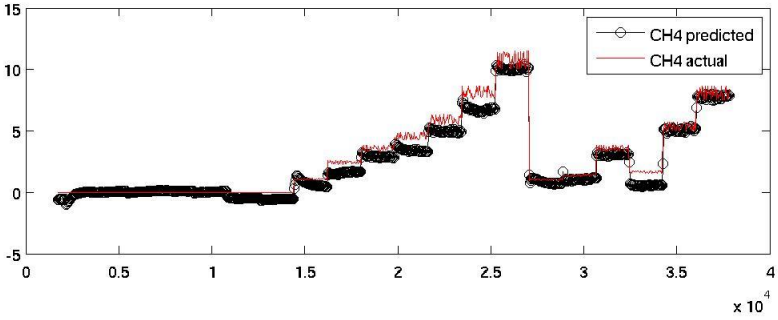
results using every 20th data point provides slightly better results than just using the steady state averages. i.e. adding more data points does appear to improve the predictions. By using every 20th data point in this example, the computation time is still reasonable (~30 seconds) and reduces the original number of lines from ~18000 to ~900. At this point, it is unclear how many data points is optimum, and that is being investigated.

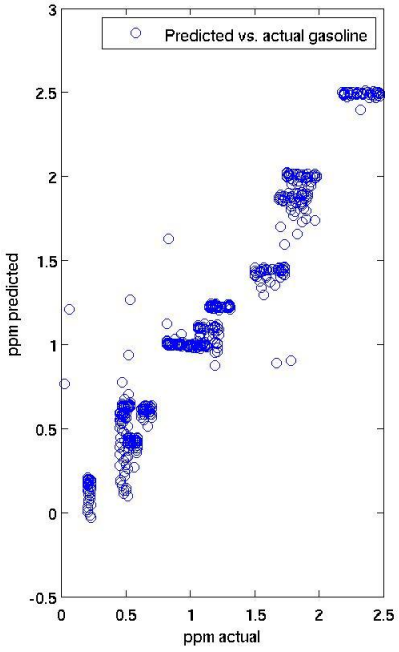


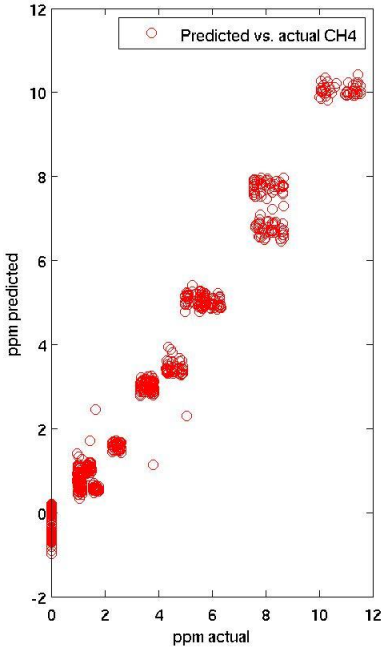

training responses
sensor R/R0
experiment time [s]
x 10^4
2600-20
2600-..
2602-37
2602-38
5121-65
5121-66
5121-67
5121-68
e2v-5525-x-CO
BM-silver

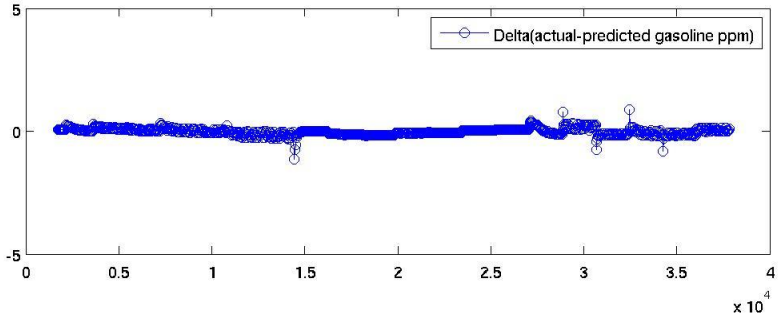

New prediction voltages
sensor R/R0
experiment time [s]
x 10^4
2600-20
2600-..
2602-37
2602-38
5121-65
5121-66
5121-67
5121-68
e2v-5525-x-CO
BM-silver

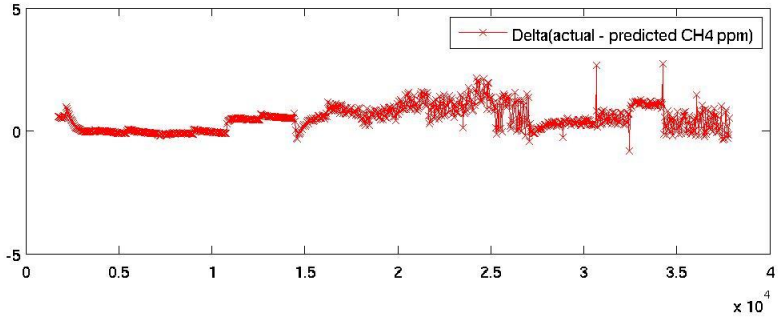

predicted gasoline ppm
actual gasoline ppm
x 10^4


CH4 predicted
CH4 actual
x 10^4


Predicted vs. actual gasoline
ppm predicted
ppm actual


Predicted vs. actual CH4
ppm predicted
ppm actual


Delta(actual-predicted gasoline ppm)
5
0
-5
0
0.5
1
1.5
2
2.5
3
3.5
4
x 10^4


Delta(actual - predicted CH4 ppm)
5
0
-5
0
0.5
1
1.5
2
2.5
3
3.5
4
x 10^4