Appendix L – Model to Monitor Comparison

1.0 The Comparison of the Monitored Ambient Concentrations at the Four Study Sites to Modeled Predicted Concentrations.

Part of the grant for the Tonawanda Community Study was to utilize the Regional Air Impact Modeling Initiative software program or RAIMI. When conducting community studies, the use of air dispersion models to predict ambient impacts is important because the costs involved of establishing monitors and analyzing data is limited by analytical test methods and overall high costs. RAIMI is more than an air dispersion model but a software program designed to review and modify data output. The RAIMI program allows the user to input multiple sources and emission scenarios to predict ambient air concentrations at various locations in the Study area. The emission inventory complied in Appendix F was invaluable data for running the RAIMI model. For a more detailed description of the RAIMI model, see Appendix I.

In section 7.1.3, the measured ambient concentrations for the study area sites were compared and evaluated to the modeled 2002 National Air Toxics Assessment data (NATA). Monitored data for Category C compounds were compared to the modeled concentration of the census tract centroid representative of the air monitoring site. Section 7.1.3 describes the procedures that were used to make these comparisons. It was determined that no further knowledge could be gained by doing similar comparisons for the 1996 NATA and 1999 NATA because of one, the age of the emission inventories, and two, the NATA modeling procedures and tools have become more refined in later years yielding a better estimation of ambient concentrations in the 2002 NATA version.

When using the RAIMI software air dispersion model to compare the model to monitored concentration data, the monitored values classified in the Study's Category C were chosen for the comparison of predicted modeled concentrations to actual monitored concentrations. In addition, for the monitoring sites, Beaver Island State Park (BISP) and Brookside Terrace (BTRS), the Category B compound, mixed xylenes, was included in the model to monitor comparison. Mixed xylenes were chosen because it is a good indicator of gasoline emissions from mobile sources and PBS transfer and storage facilities. Also, for the monitoring sites Grand Island Blvd (GIBI) and BTRS, Category B compound, 1,3,- butadiene was included in the model to monitoring comparison because 1,3,- butadiene is a good indicator of combustion decay products from mobile and point sources. At the other two monitoring sites, 1,3,- butadiene was listed in Category A and there is less valid data for a model to monitoring comparison but the data is presented.

For the model to monitoring comparison analysis, two Category C compounds were excluded from the analysis. Carbon tetrachloride and chloromethane were not part of the model to monitored comparisons because these compounds are determined to be ubiquitous nationwide at the concentrations measured at the Study area's monitors. For these two compounds, the background concentrations are estimated to be either at or

above the monitored concentration at the Study area's monitors and there are no reported localized emissions.

Also excluded from the model to monitoring analysis, were the compounds trichlorofluoromethane, trichlorotrifluoroethane and acetone. There is no data on ambient background concentrations of these compounds nor is there data of localized emissions. The emissions of acetone may be obscured because under the allowable reporting emissions procedures, acetone can be classified within the class of compounds known as total volatile organic compounds. A review of the VOC emissions from the major facilities did not uncover the use or release of acetone.

2.0 Predicted Modeled Concentrations using the RAIMI Software versus Modeled NATA 2002 Concentrations at Census Tract Centroid Level

The intention of comparing the predicted ambient concentrations from the RAIMI program with similar data from NATA 2002 is to evaluate how well the RAIMI program is performing with respect to a model that has under gone extensive peer review.

The predicted output concentrations of RAIMI at the census tract centroid were compared to the similar predictions from NATA. NATA, which uses the ASPEN model (Assessment System for Exposure Nationwide) incorporates breakdown and secondary formation of pollutants whereas the RAIMI model does not. Breakdown and secondary pollutant formation is important when modeling pollutants that are extremely reactive or modeling pollutants traveling over great distances. For our comparison between the predicted concentrations of NATA vs. RAIMI, five Category C compounds were chosen to make a model to model comparison. The goal of the model to monitor comparison is a 1:1 ratio between the two models. The compounds chosen, benzene, toluene, xylene, and acetaldehyde yielded ratios between 1:2 and 2:1. When conducting model to monitor comparisons, USEPA believes this as an acceptable outcome[1]. A scatter plot describing the relationship between the two models is presented in Table L-1.

When preparing a model to monitor or model to model comparison, the total predicted concentration can include up to five sectors, point, area, mobile including on-road and non-road and background. For the total predicted RAIMI calculated concentration, the background and non-road concentrations used in NATA were used.

For example, Table L-2 shows the predicted benzene concentrations of the two models at the nine census tract centroids. RAIMI under predicts on all occasions except for census tract 7800. This census tract centroid is located downwind of our study site; and RAIMI shows a greater point source influence.

For benzene in general, the RAIMI model under predicted for the area source sector. The contribution to the area source sector in our localized inventory did not have the number of area source categories that were modeled with NATA, source categories such as open burning, lawn mower emissions, natural emissions, etc. The complete breakdown of the

[1] USEPA, Air Toxics Data Analysis Workbook, Section 7, Advanced Analyses, June 2009

point, area and mobile source's contribution to the total concentration at the census tract centroid can be found in Table L-3

The greatest discrepancy in the ratios is the first census tract 5800, south of the Study area nearest to the city of Buffalo, and it is believed that the influence of the Buffalo area impacts raises these concentrations for NATA. Plus, this census tract is downwind of the Tonawanda industrial area missing a significant of contribution of point source emissions.

Census tract 7302 is across the Niagara River located with our upwind monitor. This is a large census tract and largely wooded. This tract would have upwind influence not captured in our Study area.

For the remaining census tracts, the two models perform within 60 to 80 percent of each other. The RAIMI model ambient air quality predictions were similar to the NATA predictions.

3.0 Predicted Modeled Concentrations using the RAIMI software versus Monitored Concentrations

The predicted modeled concentrations were calculated using the RAIMI software air dispersion model. In total, ten compounds were chosen for a model to monitoring comparison. See Table L-4 for a complete listing of model to monitoring results.

Under the National Air Toxics Assessment (NATA), model to monitor comparisons were performed to assess the reliability of the ASPEN model. As stated above, the USEPA believes that a factor of two indicates good agreement between the predicted modeled concentration value and the actual monitored concentration. To account for a model to monitor concentration for air contaminants, especially those which have many sources of emissions, including mobile sources, it is important to have an inclusive emission inventory. In the Tonawanda Air Quality Community Study, one monitored pollutant, carbon disulfide, had one large point source of emissions and a small contribution of minor emissions from other sources, with no mobile source contribution. The model to monitor ratio for carbon disulfide was in good agreement as shown below at the nearest sites:

Monitoring Site	BISP	SPWT	GIBI	BTRS
Model to Monitor Ratio	0.47	0.99	0.82	0.39
Distance (m) of Monitor to 3M	2,200	1,200	1,400	3,000

3M Tonawanda is a major source of carbon disulfide emitting over 150 TPY. The Sheridan Park Water Tower (SPWT) monitor is within 1,200 meters of 3M Tonawanda

and in the prevailing wind direction, winds from the southwest. The ratios for SPWT and GIBI are in agreement with the US EPA's target for a modeled to monitored concentration within a factor of two. The other two sites were under the one-half ratio indicating less agreement. This will be further addressed in the Bias Statistic section 4.0

When calculating the median value of the model to monitoring ratio for an air contaminant across all four monitoring sites, all sites span within a factor of two with the exception of acrolein and dichlorodifluoromethane. Acrolein, a product of combustion was most likely not properly accounted for from large combustion sources and automobiles. Dichlorodifluoromethane, with the exception of the landfills has no known reported emissions.

When comparing the range of model to monitor ratios for the individual air contaminants, the lower end of the range (under prediction) was dichlorodifluoromethane at all sites. The upper end of the range (over prediction) was mixed xylene compounds at Brookside Terrace and 1,3- butadiene at Sheridan Park Water Tower at 3.6 and 2.7, respectively.

The average ratio along with the minimum and maximum ratio is presented below for all air contaminants at each site to describe the consistency of the model at each location. The range is driven by the two compounds described below which were under predicted, acrolein and dichlorodifluoromethane.

Monitoring Site	BISP	SPWT	GIBI	BTRS
Model to Monitor Ratio Average	0.58	1.17	0.61	1.25
Minimum Ratio	0.005	0.02	0.02	0.11
Maximum Ratio	1.1	2.7	1.16	3.6

With exception of dichlorodifluoromethane and acrolein, the model to monitor ratios shows a fairly consistent trend that the model is reasonably accurate for the purposes of this study. The modeling results matched with the Beaver Island State Park monitor appears to under predict because of the lack emission source data coming from the south towards Buffalo and Lake Erie and the GIBI site appears to under predict because of the the low emissions inventory input for benzene, acrolein and formaldehyde. The Bias statistic section below allows for a mathematical approach to describe the model to monitor results.

4.0 Mean Bias Statistics and Mean Error for RAIMI Model Air Concentration Predictions and Monitored Concentrations

In air pollution science, the Mean Bias and Mean Fractional Bias calculations are used to evaluate the model to monitored paired values for criteria pollutants to determine if the model adequately reflects the observed data. Large scale regional models developed for State Implementation Planning contain hundreds of data points and similar paired results

leading to a more robust mean bias and mean error type of mathematical analysis. In the Study area, only four points (monitors) are available for mean bias and mean error reporting. Nonetheless, the results depict another way to express the model to monitor comparisons besides using only the ratio approach as discussed in section 3.0

Mean Bias (MB) and Mean Error (ME) are useful metrics for comparing the differences between modeled concentrations and monitored data but for data skewed by a couple of paired results, the use of the Mean Fractional Bias (MFB) and Mean Fractional Error (MFE) helps to better characterize the data (Boylan, et.al 2006). It is suggested by Boylan to portray both types of bias, MB and MFB, to understand the difference when using normalized or fractional bias data and error. The performance metrics for MFB is -200% to 200%, similar to the one-half to a factor 2 suggested by USEPA for model to monitor performance. The performance metric of MB and ME is zero but without the bounded statistic found with the MFB.

The results of the MB and ME calculations can be found in Table L-5. Acrolein and formaldehyde were both greater than the performance metric, -200%, -493 and -228 percent respectively for MFB indicating a gross under prediction for these two compounds. 1,3-Butadiene was within 200% for MFB but the gross Error exceeded the two hundred percent indicating specific paired values were grossly over predicted but not all the values were unacceptable.

Table L-1 Scatter Plot of RAIMI versus NATA

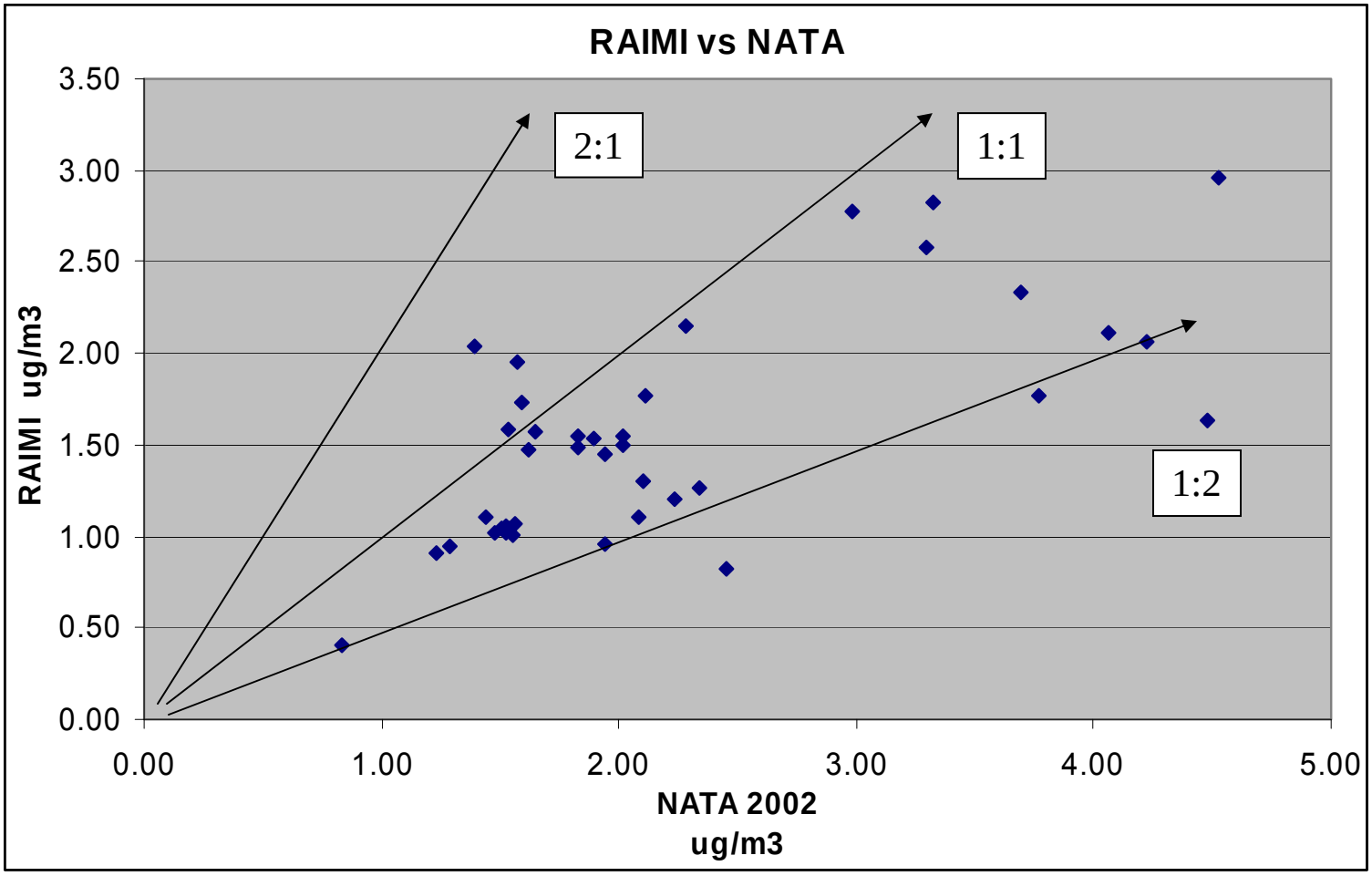


Table L-2 NATA 2002 vs RAIMI

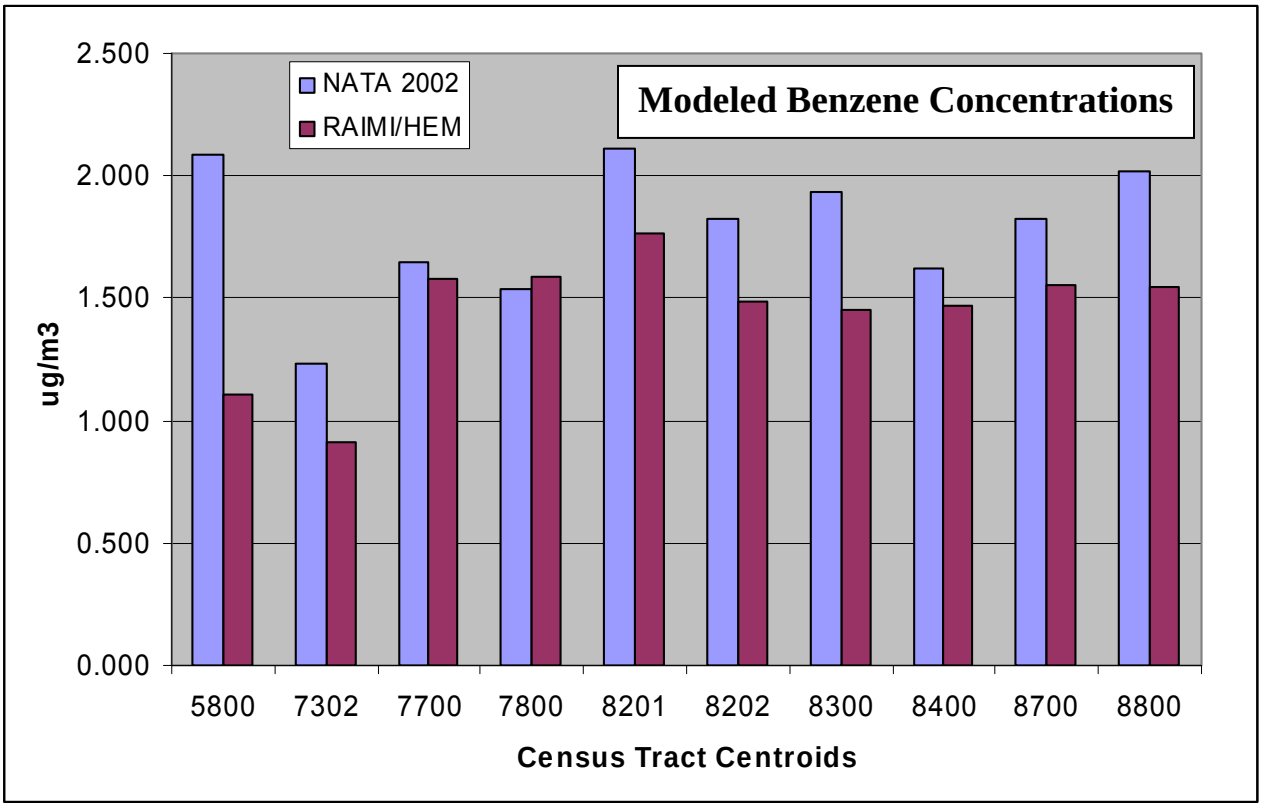
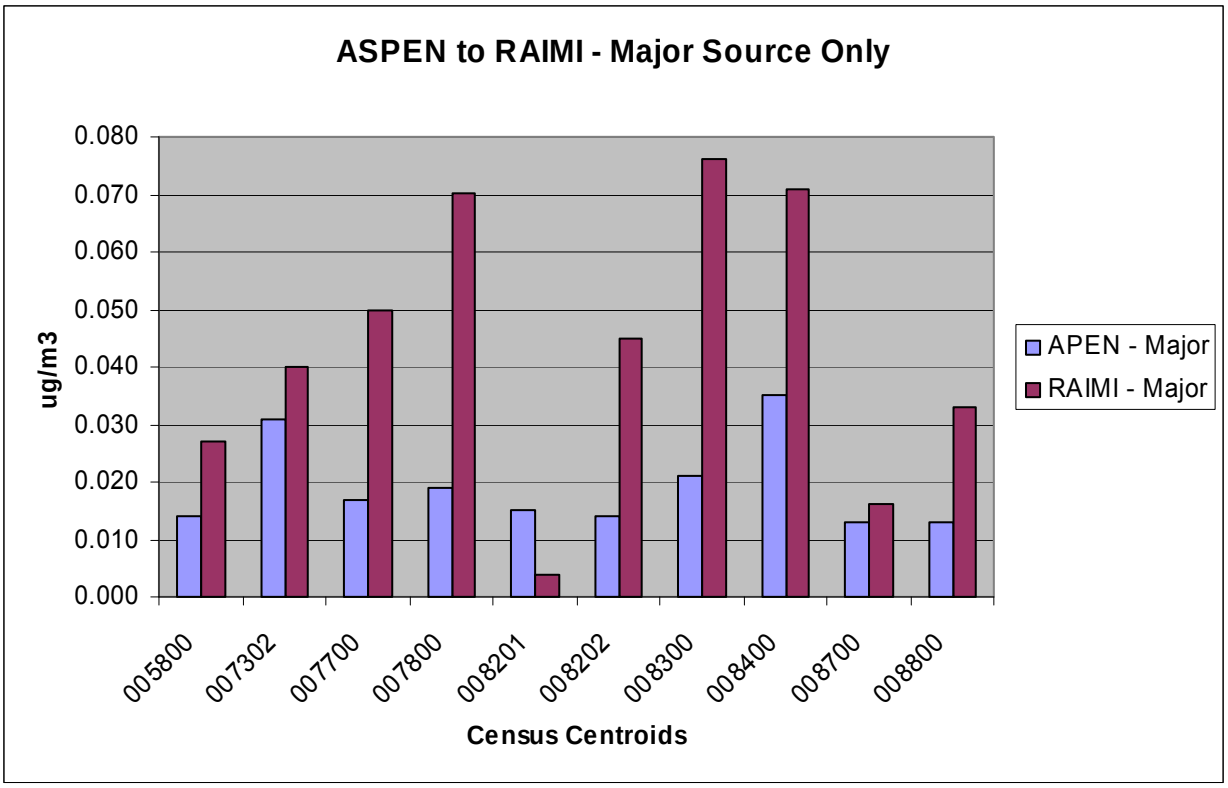
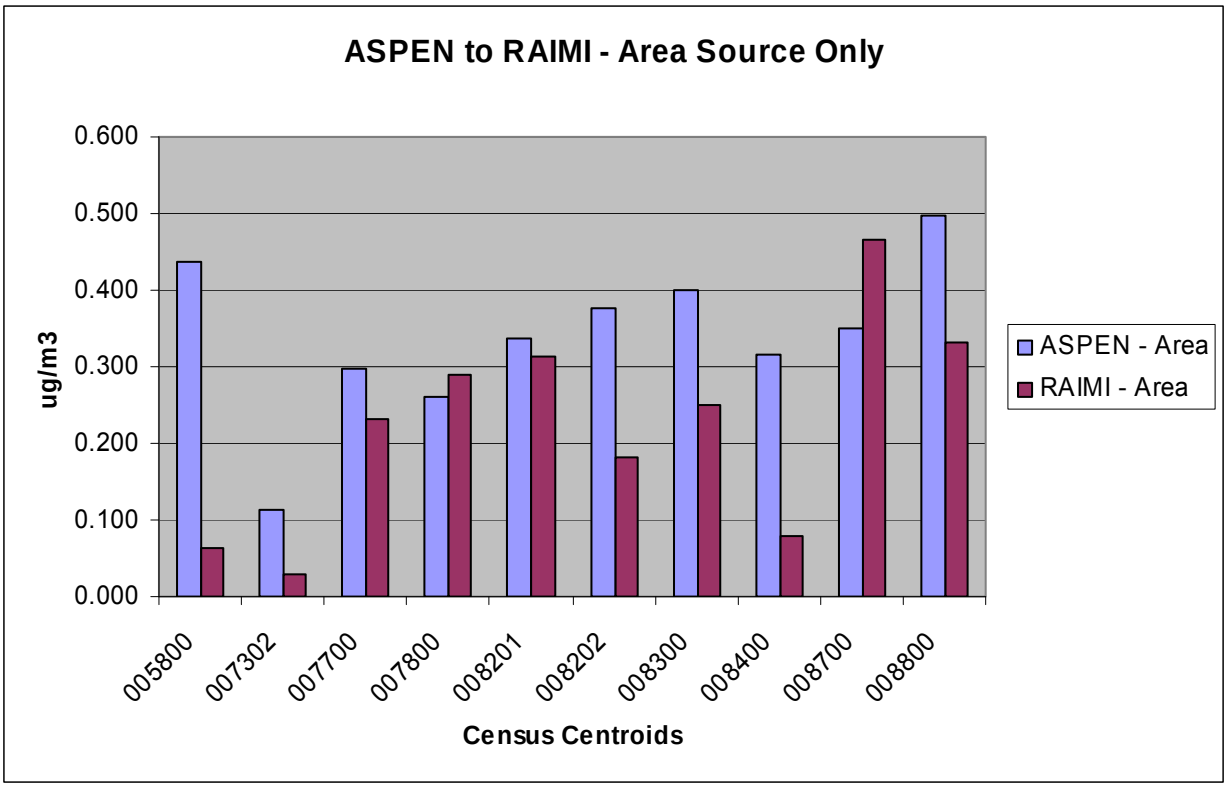


Table L-3 - Difference between Major, Area and Mobile Source Contribution on Total Concentration at Census Tract Centroid Locations - Benzene




ASPEN to RAIMI - Area Source Only
0.600
0.500
0.400
0.300
0.200
0.100
0.000
ug/m3
005800
007302
007700
007800
008201
008202
008300
008400
008700
008800
Census Centroids
ASPEN - Area
RAIMI - Area

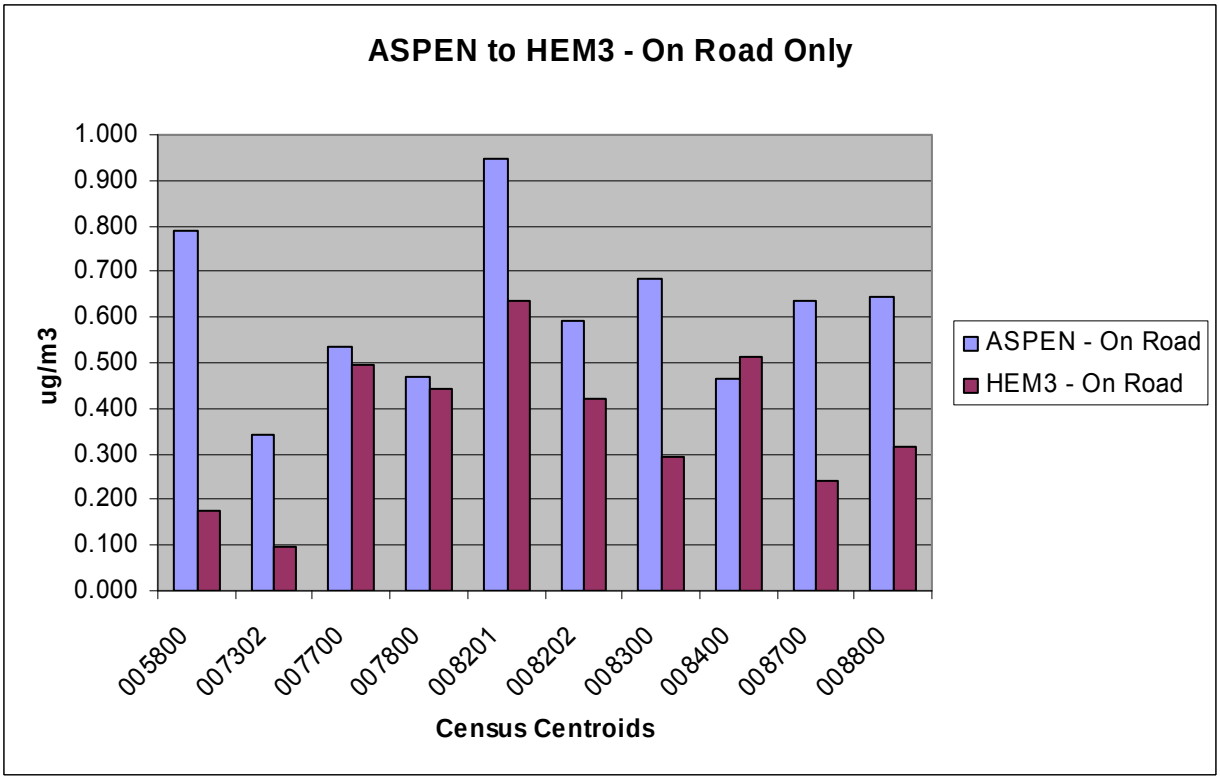

ASPEN to HEM3 - On Road Only
1.000
0.900
0.800
0.700
0.600
0.500
0.400
0.300
0.200
0.100
0.000
ug/m3
005800
007302
007700
007800
008201
008202
008300
008400
008700
008800
Census Centroids
ASPEN - On Road
HEM3 - On Road

Table L-4 - Ratio of Model to Monitoring for Selected Ten Compounds

Compounds	BISP	SPWT	GIBI	BTRS	Median	Average
Acetaldehyde	1.08	1.27	0.87	0.95	1.02	1.05
Acrolein	0.07	0.11	0.06	0.106	0.09	0.09
Benzene	0.82	1.78	0.30	1.1	0.95	0.99
1,3 Butadiene	0.99	2.68	0.61	1.79	1.39	1.51
Carbon disulfide	0.46	0.99	0.83	0.51	0.67	0.68
Dichlorodifluoromethane	0.005	0.018	0.018	0.12	0.02	0.04
Dichloromethane	0.39	1.00	1.16	1.69	1.08	1.06
Formaldehyde	0.53	0.94	0.29	0.74	0.64	0.63
Xylene - Mixed Isomers	0.52	0.77	0.98	3.58	0.87	1.45
Toluene	0.95	2.17	0.98	1.95	1.47	1.52
Average by Site	0.58	1.17	0.61	1.25		

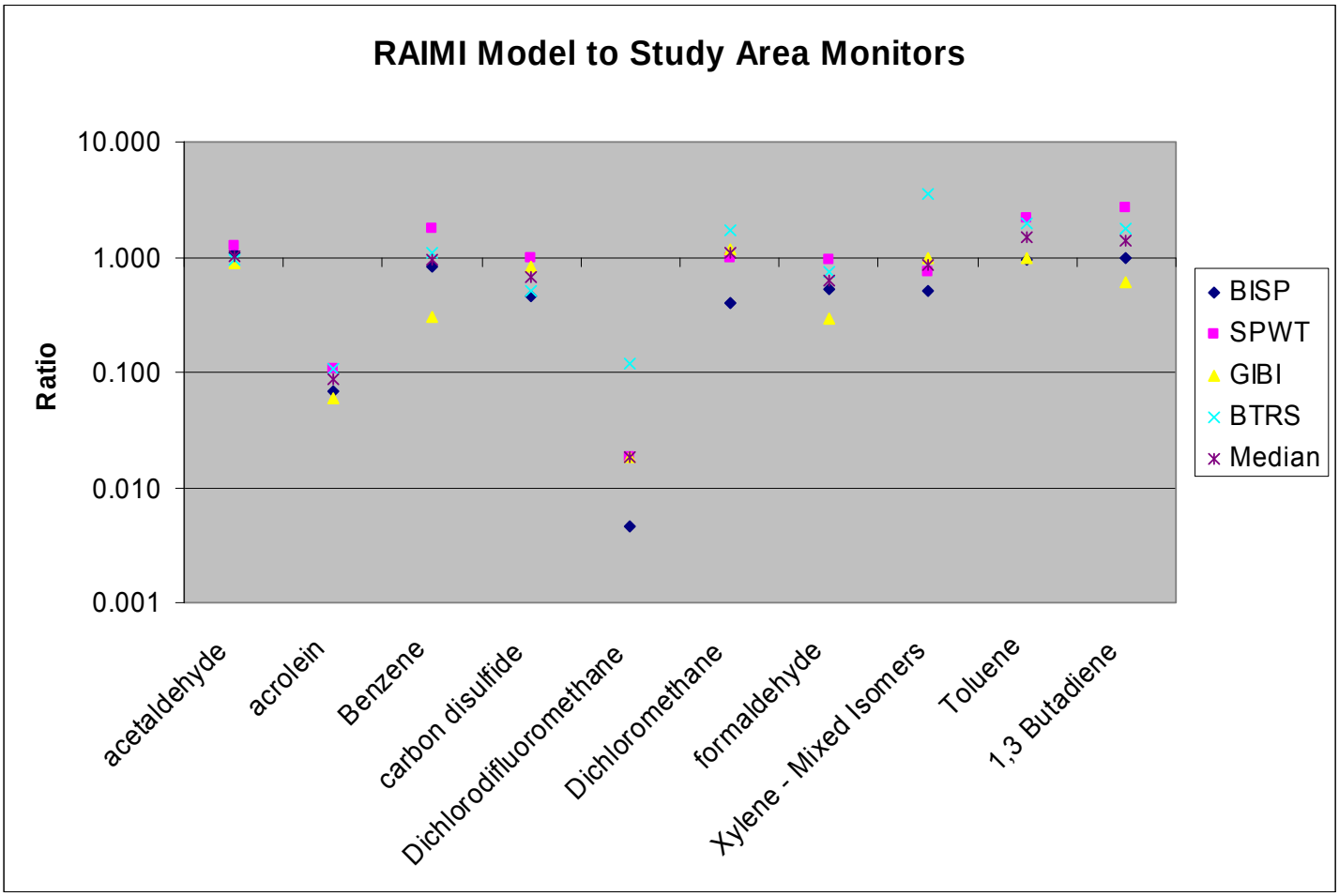


Table L-5 Mean Bias and Error Statistics

Compound	Mean BIAS	Mean ERROR	Mean Fractional BIAS	Mean Fractional ERROR
Acetaldehyde	0.03	0.14	7.4	44.4
Acrolein	-0.31	0.31	**-493.3**	**493.3**
Benzene	-1.71	1.95	-95.4	158.0
Carbon disulfide	-0.47	0.47	-155.0	155.0
Dichloromethane	0.21	0.31	169.5	213.0
Formaldehyde	-1.75	1.75	**-228.9**	**228.9**
Xylene - Mixed Isomers	0.38	0.77	49.7	142.3
Toluene	0.31	0.36	51.3	57.0
1,3 Butadiene	0.63	0.68	164.2	**263.4**

Mean Bias = 1/N ∑n (model -Obs)

Mean Error = 1/N ∑n (ABS(model -Obs))

Mean Fractional Bias Statistic = 1/N ∑n ((model -Obs)/((Obs+model)/2) * 100

Mean Fractional Error Statistic = 1/N ∑n ((ABS(model -Obs))/((Obs+model)/2) * 100