FINAL REPORT

IMPLEMENTATION AND EVALUATION OF BULK RICHARDSON NUMBER SCHEME IN AERMOD

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Prepared for

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1.0 INTRODUCTION

The AERMOD dispersion model was designed to accept a wide range of site-specific meteorological measurements, including profiles of wind, temperature and turbulence data. However, the algorithm for estimating the heat flux under stable conditions requires a cloud cover measurement, which is not typically available from site-specific monitoring programs. For applications of AERMOD in remote settings, the non-representativeness of cloud cover measurements from the nearest airport may present an obstacle to the application of AERMOD. Concerns have also been raised regarding the representativeness of cloud cover measurements from Automated Surface Observing System (ASOS) installations due to limitations in the vertical range of the ceilometer (EPA, 1997).

An alternative scheme for estimating heat flux under stable conditions based on the use of a low-level ΔT measurement together with a single wind speed measurement, referred to as the Bulk Richardson Number Scheme, has been implemented in the AERMET meteorological processor. This paper presents results of a technical review and modification of the implementation of the Bulk Richardson Number Scheme in AERMET, and results of an evaluation of the AERMOD model performance using the modified Scheme as compared to the use of cloud cover data.

2.0 RESULTS OF AERMET REVIEW

2.1 ISSUES WITH CURRENT IMPLEMENTATION

A review of the current implementation of the Bulk Richardson Number Scheme in AERMET (dated 02222) (Cimorelli, *et al*., 2002) identified a number of issues that could significantly affect the results of applying the Scheme. The current implementation involves an iterative solution to estimate the surface friction velocity ($u*$), the temperature scale ($\theta*$), and the Monin-Obukhov length (L), based on the reference wind speed and ΔT if the wind speed is above a critical wind speed. The original implementation was designed to linearly extrapolate $u*$ and $\theta*$ for wind speeds below the critical wind speed. However, the method was implemented in version 02222 without the extrapolation, and the values of $u*$ and $\theta*$ evaluated at the critical wind speed were used for wind speeds below the critical value.

An effort was made to resolve the issues associated with the current implementation of the Scheme in AERMET, and a revised version of the code was developed, referred to hereafter as version 02222R. However, once the initial issues with the current implementation were resolved, additional issues with the performance of the Scheme were encountered during tests with the Prairie Grass tracer field study data (Barad, 1958; Haugan, 1959). In particular, cases were encountered where the wind speed was initially above the critical wind speed, but fell below the critical wind speed during the iteration as the critical wind speed was adjusted. The current implementation in version 02222 assigns such cases as missing. In preliminary tests of the revised version (02222R), using the Prairie Grass data, the top three observed and predicted concentrations (based on cloud cover data) fell into this category.

2.2 ALTERNATIVE IMPLEMENTATION METHODS

Given the number of issues encountered with the current implementation of the Scheme in AERMET, and in particular the issues associated with wind speeds below the critical wind speed, alternative implementation options were explored. One of the methods considered was the "profile method" (van Ulden and Holtslag, 1985; Nieustadt, 1978; McBean, 1979; and Berkowicz and Prahm, 1982). This method consists of making an initial estimate of L, calculating u^* and θ^* from the profile equations for wind and temperature based on similarity theory, then calculating a new estimate of L based on u^* and θ^* and iterating to a solution. This method provides a straight-forward approach without any critical wind speed issue. The equations for u^*, θ^*, and L are as follows:

$$u_* = \frac{k\,u}{\left[\ln\left(\frac{z}{z_0}\right) + \frac{\beta_m z}{L}\right]} \tag{1}$$

$$\theta_* = \frac{k\,\Delta\theta}{\left[\ln\left(\frac{z_2}{z_1}\right) + \frac{\beta_m\,(z_2 - z_1)}{L}\right]} \tag{2}$$

$$L = \frac{T_{ref}\,u_*^2}{k\,g\,\theta_*} \tag{3}$$

where

β_m = profiling constant (= 5)

k = von Karman constant (= 0.4)

g = acceleration due to gravity (= 9.8 m/s^2)

u = wind speed at height z (m/s)

z = measurement height above ground (m)

z_0 = surface roughness length (m)

θ = potential temperature at height z (K)

$\Delta\theta$ = potential temperature difference between heights z_2 and z_1 (K)

In this implementation of the profile method, the level of the wind speed measurement used in Equation 1 is independent of the measurement levels used for ΔT. The method was implemented in AERMET to use the reference wind speed, defined as the lowest valid wind speed measurement from a level at or above $7z_0$ and less than or equal to 100m. The method was also implemented using a tolerance of 1 percent on the estimates of $u*$, $\theta*$, and L.

The initial implementation using the profile method provided encouraging results for the Prairie Grass database, with convergence typically occurring within about 5 iterations. However, the method did not converge well on other test databases, resulting in large numbers of cases with values of 0 (zero) for $u*$.

One of the alternative options considered was a program developed by John Irwin (Irwin and Binkowski, 1981) that implements the profile method using a different iteration scheme. The Irwin code makes an initial estimate based on a neutral lapse rate, and then iterates in a stepwise manner with successive estimates for L until the estimate overshoots the true value. Then the stepping direction is reversed and the stepping interval is reduced until convergence is achieved. A lower limit of z/2 is placed on the value of L, where z is the height of the wind speed measurement. The Irwin code (hereafter referred to as the Prof_LIM method to reflect the lower limit on L) also includes a modification to the wind speed profile for cases when $z/L > 0.5$ based on Holtslag (1984), expressed in terms of $u*$ as follows:

$$u_* = \frac{k\,u}{\left[\ln\left(\frac{z}{z_0}\right) + 7\ln\left(\frac{z}{L}\right) + \frac{4.25}{(z/L)} - \frac{0.5}{(z/L)^2} + \frac{\beta_m}{2} - 1.648\right]} \qquad (4)$$

Note that Equation 4 matches the result from Equation 1 for a value of $z/L = 0.5$. The Prof_LIM Method produced reasonable results for the Prairie Grass data and also appeared to provide reasonable results for other test databases.

When the original implementation of the profile method was modified to include the wind speed profile for cases when $z/L > 0.5$ based on Equation 4, the modified method continued to perform well on Prairie Grass data, but also provided reasonable results for other test databases. The original implementation of the profile method was not modified to include a lower limit on the value of L, and is referred to hereafter as the Prof_UNL method. The results of the Prof_LIM and Prof_UNL methods differed significantly for many cases in the Bulk Richardson Number test case for AERMET provided on EPA's Support Center for Regulatory Air Models (SCRAM) website (referred to as EX05), especially for very stable cases with relatively low values of L and low wind speeds. The Prof_LIM and Prof_UNL methods also produced significantly different results compared to version 02222R.

2.3 IMPLEMENTATION IN AERMET CODE

The alternative method for determining $u*$, $\theta*$, and L based on wind speed and low-level ΔT has been implemented in the AERMET meteorological processor. The iterative approach involves initial estimates of $u*$, $\theta*$, and L followed by an iterative solution of Equations 1 through 4. A minimum of 3 and maximum of 20 iterations are used to estimate $u*$, $\theta*$, and L, and a convergence criterion of 1 percent is applied simultaneously on all three parameters.

The AERMET meteorological processor was also modified to remove the dependence on cloud cover for the decision on whether a particular hour is convective or stable when solar radiation measurements are available. Version 02222 of AERMET calculates an equivalent solar elevation angle based on the solar radiation measurement, and compares the equivalent solar elevation angle to a critical angle to determine if the hour is convective or stable. However, the calculation of the equivalent solar elevation angle and the critical angle are both dependent on cloud cover, and if cloud cover is missing a value of 5 tenths is used. To circumvent this issue, an equivalent cloud cover is calculated based on the solar radiation measurement and the actual solar elevation angle for the hour, using an equation for solar radiation as a function of cloud cover and the clear sky insolation from Kasten and Czeplak (1980). The equation for equivalent cloud cover (n_{eq}) is as follows:

$$n_{eq} = \left(\frac{1 - R/R_0}{0.75} \right)^{1/3.4} \tag{5}$$

where

R = solar radiation (W/m^2)

R_0 = clear sky insolation = 990 sin(ϕ) – 30

ϕ = solar elevation angle

Cloud cover is also used in dry deposition calculations in the AERMOD model. Therefore, if cloud cover is missing during stable hours and the Bulk Richardson Number Scheme is being used, then an equivalent cloud cover is calculated based on the value of $\theta*$ calculated from the Bulk Richardson Number Scheme. The equivalent cloud cover is calculated as follows, based on van Ulden and Holtslag (1985):

$$n_{eq} = \left(\frac{1 - \theta_* / 0.09}{0.5} \right)^{0.5} \qquad (6)$$

3.0 PREDICTED VS. OBSERVED WIND SPEED AND ΔT COMPARISONS

3.1 COMPARISONS USING SCRAM TEST CASE

In order to determine whether any of the three versions of AERMET (the "corrected" version 02222R, the Prof_LIM method, and the Prof_UNL method) performed any better than the others in estimating the boundary layer parameters, a series of tests were performed to compare the wind speed and ΔT values back-calculated based on the estimates of $u*$, $\theta*$, and L to the values of wind speed and ΔT input to the routines. The SCRAM test case (EX05), consisting of one month of site-specific data from Allentown, PA, was used for the initial test. The EX05 test case includes a 10-2m ΔT and a 30m reference wind speed as inputs to the Bulk Richardson number (BulkRi) option.

The results of the wind speed comparisons based on the EX05 test case are shown in Figures 1 through 4 for the 02222R, Prof_LIM and Prof_UNL methods, along with the current version of AERMET (dated 02222). The ΔT comparisons for these four methods are shown in Figures 5 through 8. The Prof_UNL method (Figures 3 and 7) performed very well on this test, with differences in observed vs. predicted wind speed and ΔT on the order of 0.1 percent or less. Version 02222R tended to overestimate the wind speed and underestimate the ΔT, while the Prof_LIM method showed some improvement relative to version 02222R for wind speed but still showed some overestimation, and showed a more significant overestimation for ΔT. The current implementation in AERMET (version 02222) exhibits significant overprediction of wind speed and ΔT. Not surprisingly, the algorithms tended to provide better agreement between observed and predicted wind speed and ΔT for the more neutral/high wind speed cases than for the stable/low wind speed cases.

The overestimation of the input value of ΔT by the Prof_LIM method (see Figure 6) appears to be due primarily to the inclusion of the lower limit on the computed value of L to be greater than z/2. In the EX05 test case, z is equal to 30m. This limit is based on the assumption that the profile equations based on similarity theory are applicable up to a height of about L. As noted earlier, this limit on the value of L was not incorporated into the Prof_UNL method. Inclusion of this limit in the Prof_UNL method produced results very similar to those shown for the Prof_LIM method. Aside from the limit on L, the two implementations of the profile method appear to produce nearly equivalent results. Holtslag (1984) suggests that the profile equations (including Equation 4) apply reasonably well for the very stable cases up to a height of about 6z, based on data from the 213m Cabauw tower.

The results of this and other tests suggest that the profile method is fairly robust in solving the wind and temperature profile equations iteratively, without a prescribed limit placed on L, with the modification to the wind speed profile based on Equation 4. The Prof_UNL method also requires fewer iterations to converge than the Prof_LIM method, by almost a factor of 10. However, the question remains as to whether the estimates of $u*$, $\theta*$, and L from the Prof_UNL method perform any better at predicting wind speeds and temperatures at measurements heights other than those input to the method.

3.2 COMPARISONS USING KANSAS AND PRAIRIE GRASS DATABASES

Data from the Kansas (Izumi, 1971) and Prairie Grass (Barad, 1958; Haugan, 1959) field studies were used to examine the question of how well the two profile methods perform at predicting the full profiles of wind speed and temperature. The Kansas field program, conducted in 1968 at a site about 75km southwest of Dodge City, includes wind speed and temperature measurements at heights of 2, 4, 8, 16, 22.6, and 32m above ground. The Prof_LIM and Prof_UNL methods were applied for the Kansas database using the 2m reference wind speed and 8-2m ΔT. Figure 9 shows the predicted vs. observed wind speed for the Prof_LIM and Prof_UNL methods for the Kansas data, and Figure 10 shows the predicted vs. observed values of ΔT.

Of the nine hours of stable cases examined for the Kansas database, the Prof_LIM and Prof_UNL methods estimated nearly identical values of $u*$, $\theta*$, and L for eight of the cases. The results differed significantly for the most stable case, hour 0 of day 209, due to the lower limit on L for Prof_LIM. Both methods estimated a value for L of about 1m, but the Prof_UNL method estimated a value for *u** of about 0.05 m/s compared to a value of 0.09 m/s for the Prof_LIM method. The Prof_LIM method overestimates the wind speed for this case by about a factor of 2, and also overestimates the value of ΔT for this case by a factor of about 4.5.

Figure 11 shows the full profile of predicted vs. observed wind speeds for the day 209, hour 0 case, and Figure 12 shows the predicted vs. observed profiles of potential temperature gradient, (plotted at the midpoint of the height ranges). The Prof_UNL method matches the observed wind speed profile up to a height of about 8m, but starts to underestimate the wind speed above that level. The Prof_LIM method overestimates the wind speed across the full range of measurement heights. The Prof_UNL method matches the potential temperature gradient at the lowest height range of about 5m, and overestimates the lapse rate slightly above that level. The Prof_LIM method overestimates the lapse rate by about a factor of 5. These limited results suggest that use of the profile method without applying a lower limit on the value of *L* does not adversely affect the performance of the Scheme.

Similar tests were performed using the Prairie Grass database, which includes wind speed and temperature measurements at heights of 1, 2, 4, 8, and 16m above ground. A 1m reference wind and 8-1m ΔT were used. The results showing predicted vs. observed reference wind speed and input ΔT are provided in Figures 13 and 14, respectively. As with the Kansas results, the Prof_LIM and Prof_UNL methods produced nearly identical results, except for the most stable, low wind speed cases. For Prairie Grass, there were six cases that showed disparities. Of these six cases, the most stable case occurred on July 22 at hour 20, with both methods estimating values for *L* of about 0.5m, but the Prof_UNL method estimating a value of 0.03 m/s for *u** compared to a value of 0.07 m/s for Prof_LIM. The predicted vs. observed profiles of wind speed and ΔT for this case are shown in Figures 15 and 16, respectively. The results for this case at Prairie Grass are similar to the results shown above for Kansas, with the Prof_UNL method matching the full profiles better than the Prof_LIM method. An additional test was performed on the sensitivity of the results to the level of wind speed measurement used as input to the Scheme for the July 22, hour 20 case at Prairie Grass, using the 8m wind speed instead of the 1m wind speed. The results of the predicted vs. observed wind speed profiles for this test are shown in Figure 17. Comparing Figure 17 to Figure 15 suggests that the algorithm performs reasonably well regardless of the wind speed measurement height.

4.0 PRAIRIE GRASS PERFORMANCE EVALUATION

Given the results of these comparisons of predicted to observed wind speed and ΔT, the Prof_UNL method was selected for implementation in the AERMET code. The performance of the Prof_UNL method was further evaluated by comparing predicted to observed concentrations using the Prairie Grass tracer database. Given the use of the Prairie Grass data in testing different methods for implementing the Bulk Richardson Number Scheme in AERMET, Prairie Grass is considered a developmental database for this performance evaluation.

The results of the performance evaluation for Prairie Grass are shown in Figure 18 in the form of a Quantile-Quantile (Q-Q) plot for stable hours only. The Q-Q plot is generated by plotting the predicted vs. observed concentrations by rank, unpaired in time and space. The individual concentrations used in the Q-Q plot are the maximum hourly values predicted or observed along each of the five sampling arcs, located at downwind distances of 50, 100, 200, 400, and 800 meters. Figure 18 shows that the results based on the Prof_UNL method and results based on use of cloud cover data are nearly identical, and exhibit very good agreement between observations and predictions. Figure 19 shows the Q-Q plot for Prairie Grass based on using the Bulk Richardson Number Scheme in the current version of AERMOD dated 02222. The results for version 02222 show some underprediction near the peak of the distribution, and more significant overprediction for the lower part of the distribution.

In addition to the Q-Q plot, another statistic used in evaluating the performance of regulatory dispersion models is the Robust Highest Concentration (RHC), defined as an exponential tail fit to the upper end of the concentration distribution (Cox and Tikvart, 1990). The use of the RHC for model performance evaluations is intended to mitigate the impact that outliers in the database may have on evaluation results. The RHC is calculated as follows:

$$RHC = \chi\{n\} + \left(\overline{\chi} - \chi\{n\}\right)\ln\left(\frac{3n-1}{2}\right) \qquad (7)$$

where n = Min (m_o, m), m_o is the number of values used to characterize the upper end of the concentration distribution, m is the number of values exceeding a specified threshold value, $\overline{\chi}$ is the average of the n - 1 largest values, and $\chi\{n\}$ is the n^{th} largest value. The value of m_o is normally taken to be 26 except for databases with a limited sample size. The ratio of predicted to observed RHCs is 0.87 for the Prof_UNL method compared to the RHC ratio based on use of cloud cover data of 0.89. The RHC ratio based on the BulkRi Scheme in version 02222 is 0.77.

5.0 CINDER CONE BUTTE PERFORMANCE EVALUATION

Additional evaluations of the Prof_UNL method were performed using the Cinder Cone Butte (CCB) complex terrain tracer study (Strimaitis, et al., 1988) as an independent database. The CCB field study was conducted by EPA in 1980 as part of the development of the Complex Terrain Dispersion Model (CTDM), and included tracer releases of SF_6 and Freon from several release heights near an isolated hill southeast of Boise, Idaho. The results presented here are based on the SF_6 data, which consisted of 100 hours of stable meteorology for a range of release heights. The meteorological inputs to the BulkRi Scheme included a 10-2m ΔT and a 2m reference wind speed. Multiple levels of wind, temperature and σ_θ data were also available from the 150m instrumented tower. A single level of σ_w data near the height of each release was also included in the meteorological database.

The results of the evaluation for the SF_6 tracer releases are shown in Figure 20 in the form of a Q-Q plot of the hourly maximum predicted normalized concentrations (χ/Q) based on the BulkRi Scheme compared to results based on the use of cloud cover (CCVR). The plot shows very good agreement between the BulkRi and CCVR results. A more challenging comparison is provided in Figure 21, which compares the hourly maximum predicted concentrations paired in time based on BulkRi and CCVR. This plot also shows very good agreement between the two methods, especially for the upper half of the distribution. Figure 22 shows a Q-Q plot of hourly maximum predicted vs. observed concentrations using the BulkRi Scheme. The CTDM model results are also included in Figure 22 for comparison. The AERMOD model using the Prof_UNL method overpredicts the peak concentration by about a factor of 2 for this dataset, but otherwise shows good agreement with the CTDM model and with observations. This tendency for overpredicting the peak concentration is also reflected in the predicted/observed RHC ratios of 1.35 for AERMOD and 1.05 for CTDM. For comparison, the CCB SF_6 evaluation results based on version 02222 of AERMET are shown in Figure 23, which exhibit an underprediction by about a factor of 2. The predicted/ observed RHC ratio for version 02222 is 0.40.

Since the CCB database includes site-specific measurements of vertical turbulence (σ_w) near the release height, additional model comparisons were made without the observed σ_w data to ensure that the good performance of the model relative to observed concentrations was not dependent on these σ_w observations. Figures 24 and 25 show Q-Q plots of observed vs. predicted normalized concentrations for CCB for the BulkRi Scheme and CCVR, respectively, without the observed σ_w data. Figure 24 shows that model performance is actually improved somewhat, with less overprediction for the peak hours, for the BulkRi Scheme without observed σ_w. Figure 25 shows similar results for CCVR, except for the overall peak value, which shows more overprediction without the observed σ_w data. The predicted/observed RHC ratios without observed σ_w data are 1.22 for the BulkRi option and 1.64 for CCVR.

6.0 CONCLUSIONS

The modifications to the implementation of the Bulk Richardson Number Scheme in AERMET appear to have improved the performance of the AERMOD modeling system in relation to the current version of AERMET (dated 02222) based on comparisons of observed to predicted concentrations for the Prairie Grass and CCB tracer field studies. The revised BulkRi implementation produces results that are comparable to results based on the use of cloud cover data for both the Prairie Grass and CCB databases. The revised implementation also shows improved results relative to version 02222 when comparing observed to predicted wind speed and ΔT data. The modified Scheme based on the Prof_UNL method appears to provide a robust method for estimating boundary layer parameters under stable conditions when representative cloud cover data are not available, using a single wind speed measurement and a low-level ΔT.

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Figure 1. Observed vs. Predicted Wind Speed - Version 02222R

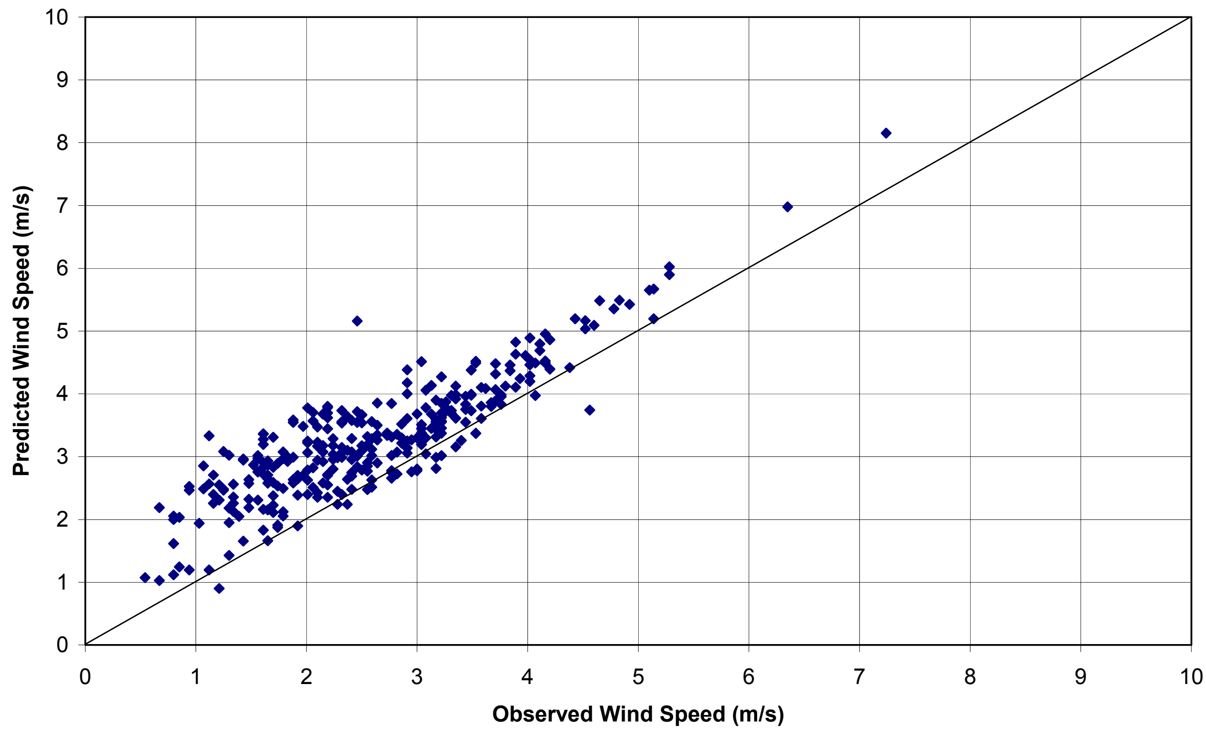

Figure 2. Observed vs. Predicted Wind Speed - Prof_LIM Method

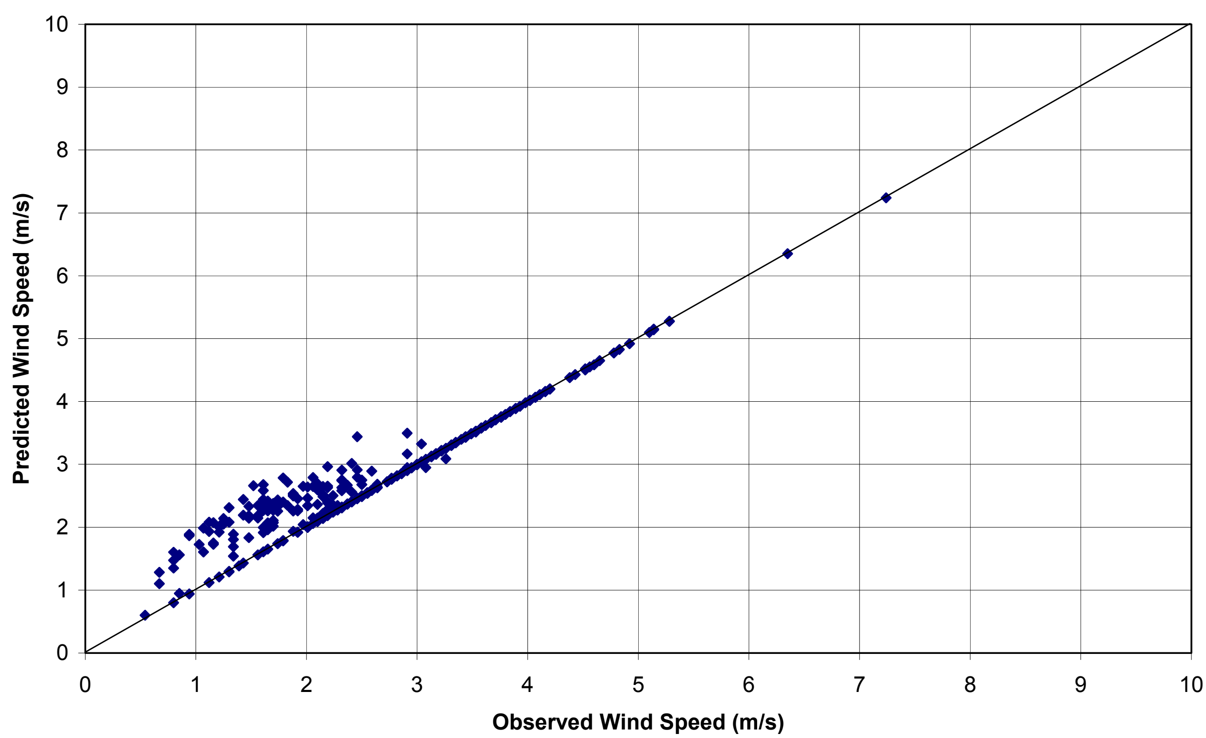

Figure 3. Observed vs. Predicted Wind Speed - Prof_UNL Method

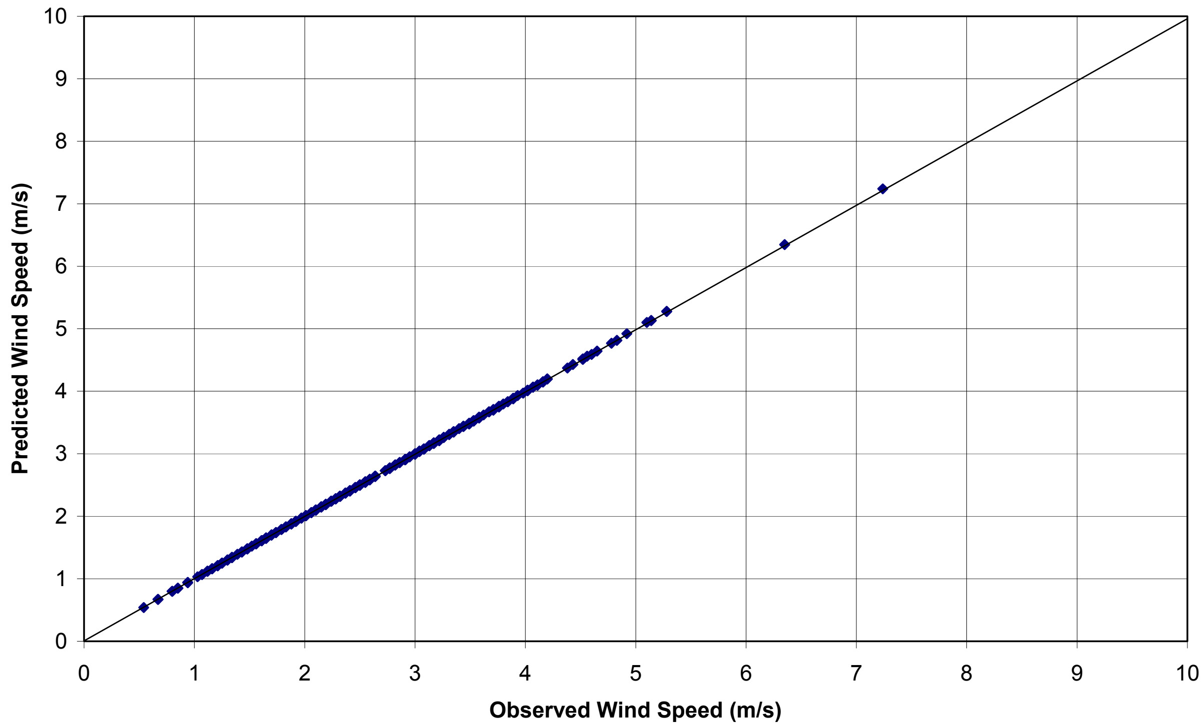

Figure 4. Observed vs. Predicted Wind Speed - Version 02222

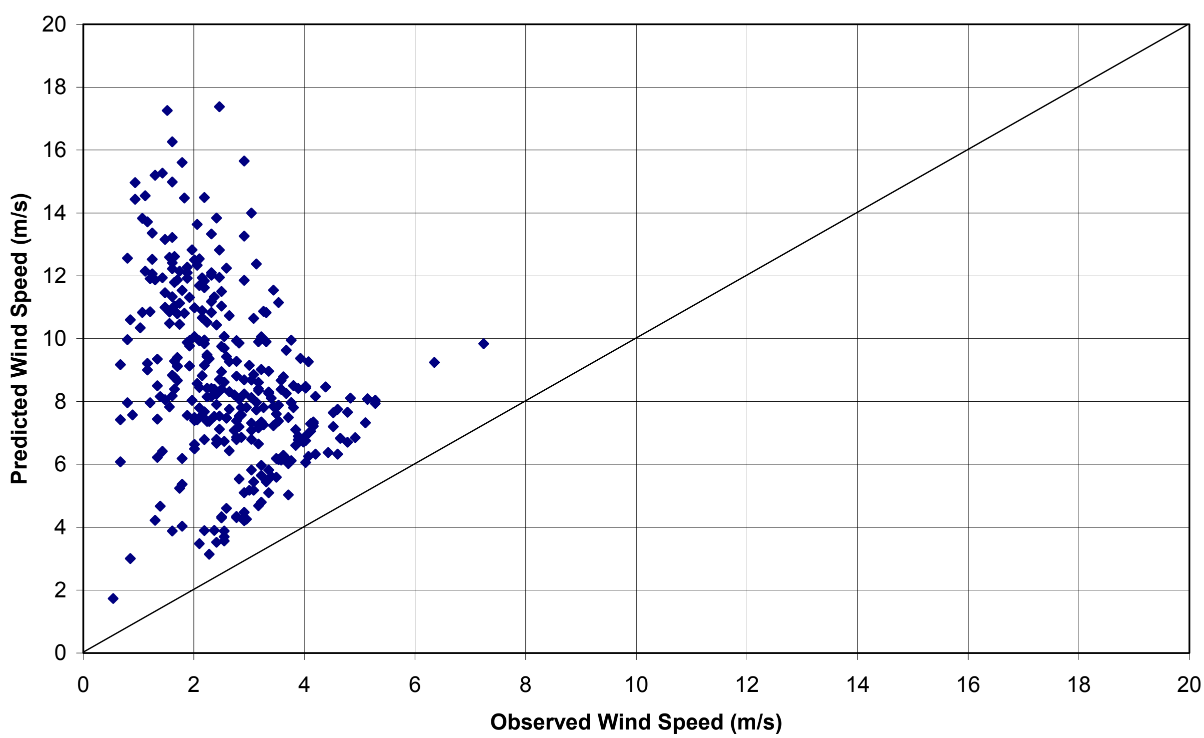

Figure 5. Observed vs. Predicted ΔT - Version 02222R

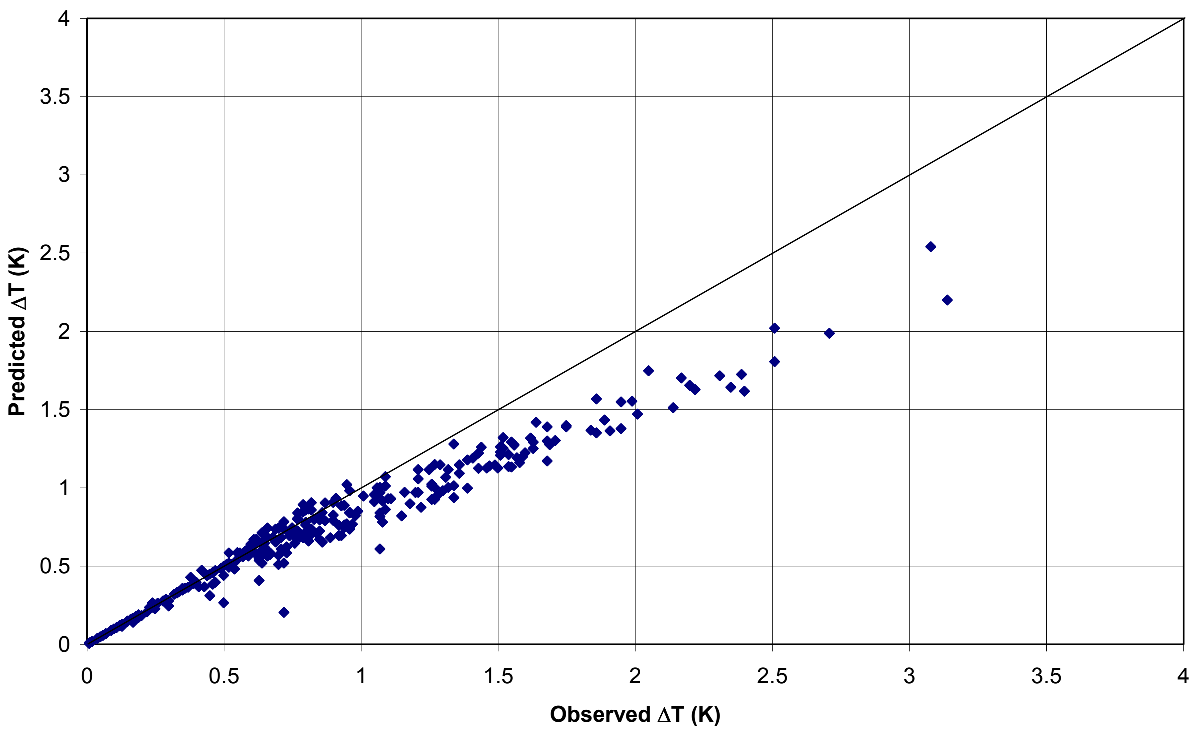

Figure 6. Observed vs. Predicted ΔT - Prof_LIM Method

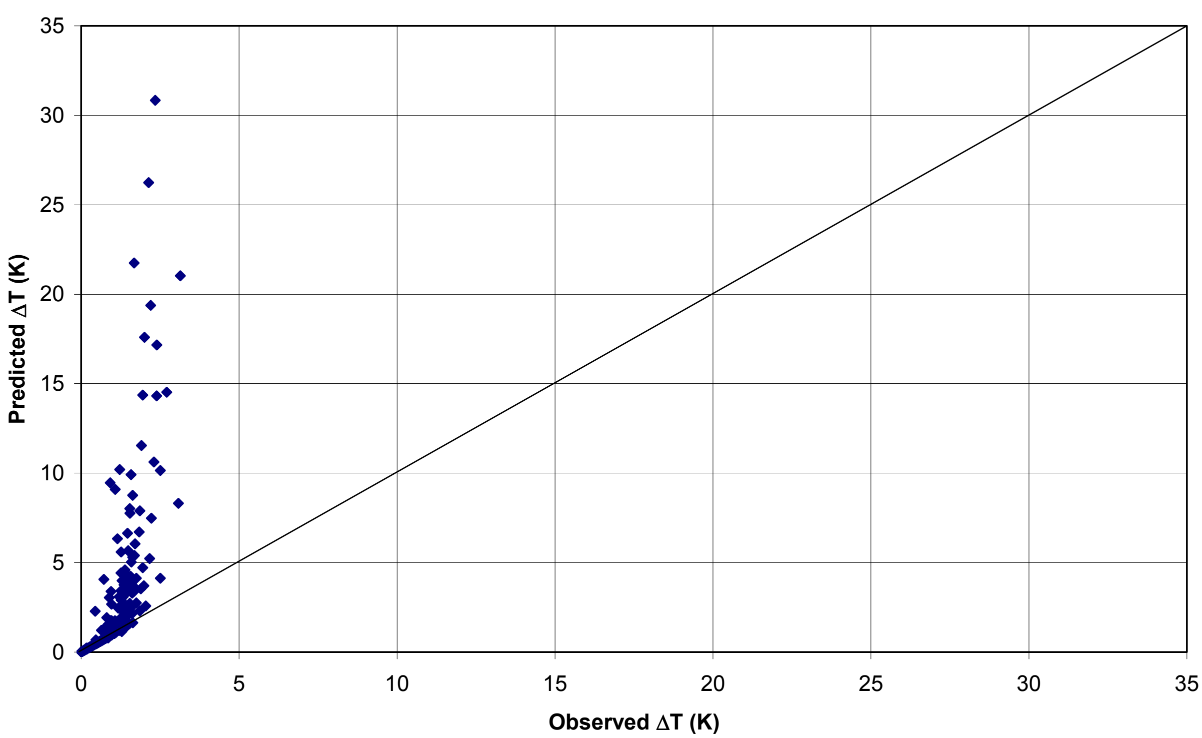

Figure 7. Observed vs. Predicted ΔT - Prof_UNL Method

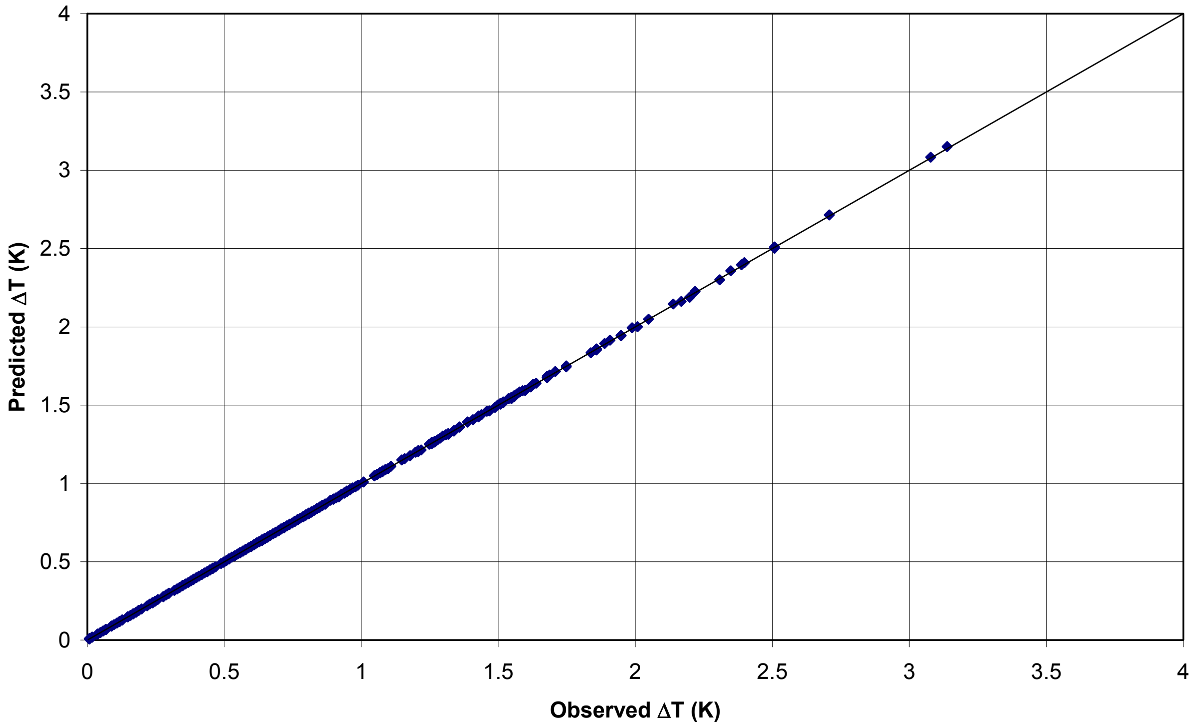

Figure 8. Observed vs. Predicted ΔT - Version 02222

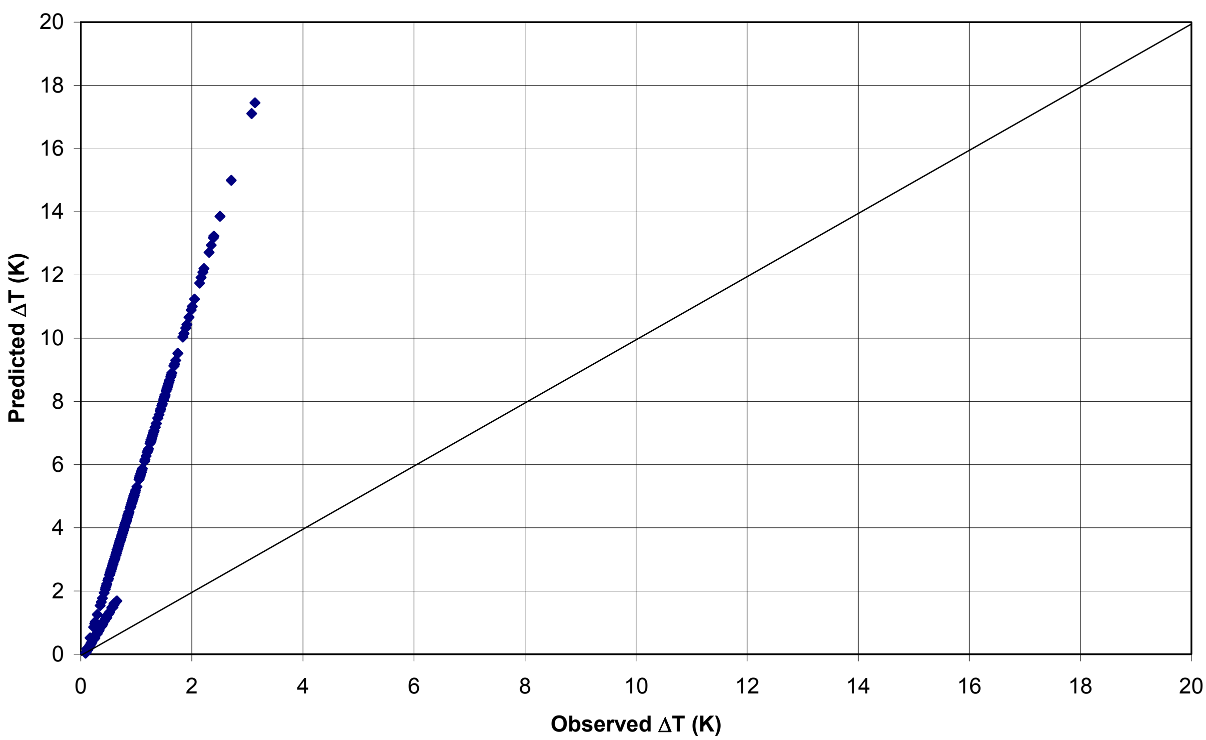

Figure 9. Comparison of Predicted to Observed Wind Speed for Kansas Data

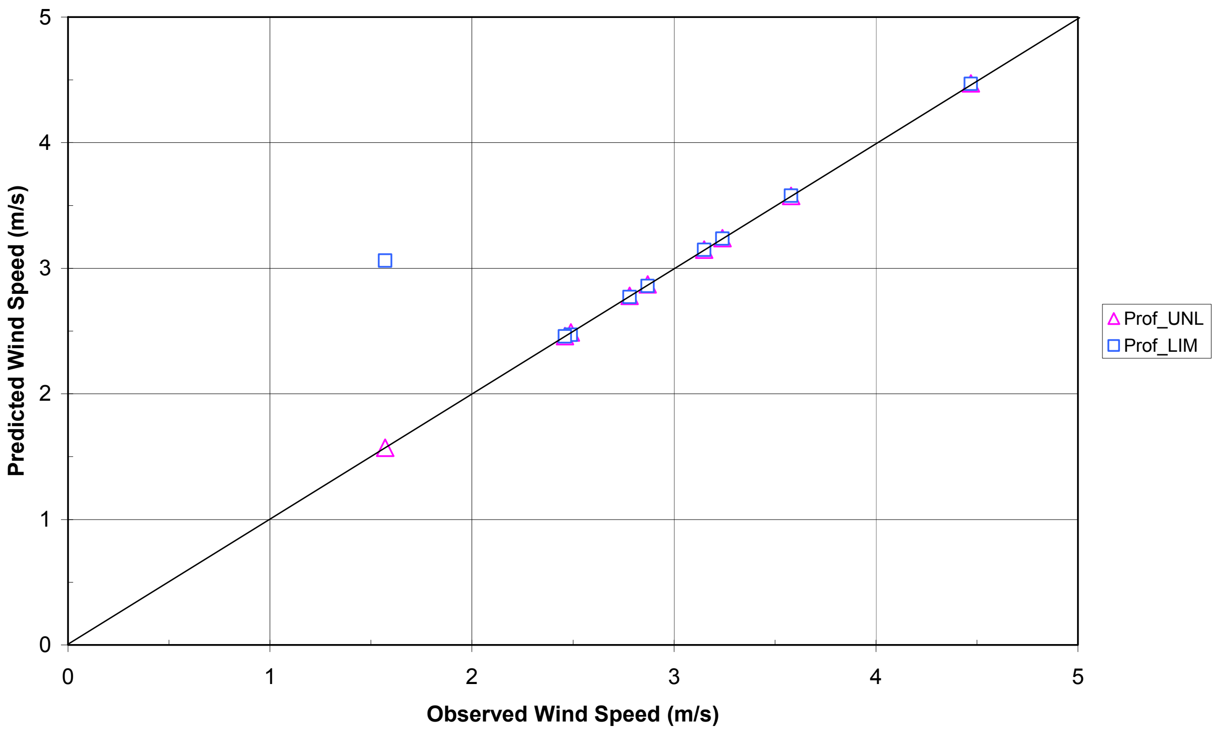

Figure 10. Comparison of Predicted to Observed ΔT for Kansas Data

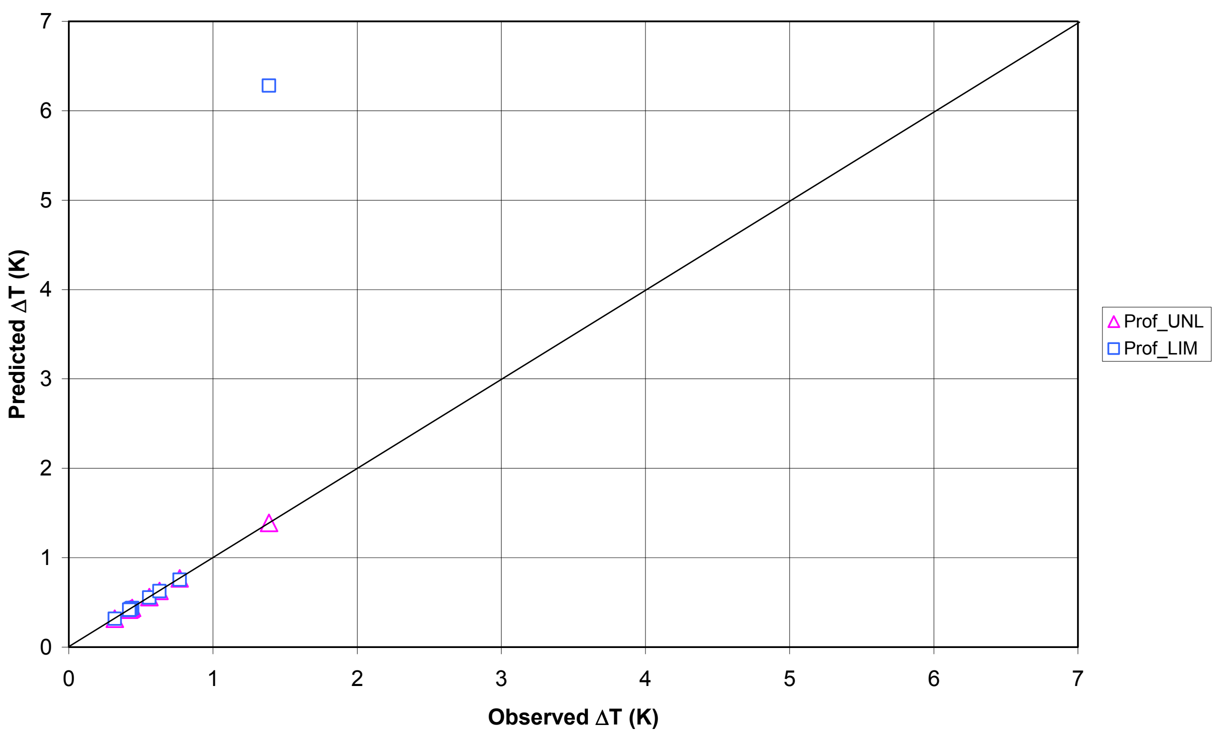

Figure 11. Observed vs. Predicted Wind Speed Profiles - Kansas, Day 209, Hour 0

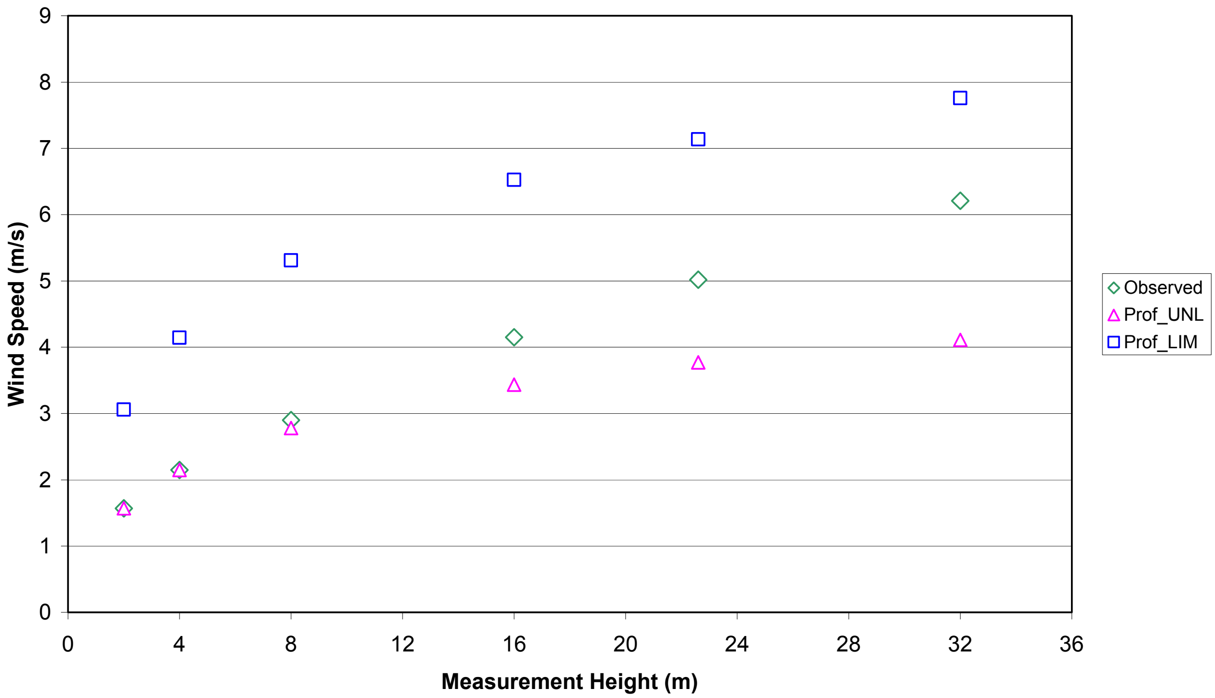

Figure 12. Observed vs. Predicted Δθ/ΔZ Profiles - Kansas, Day 209, Hour 0

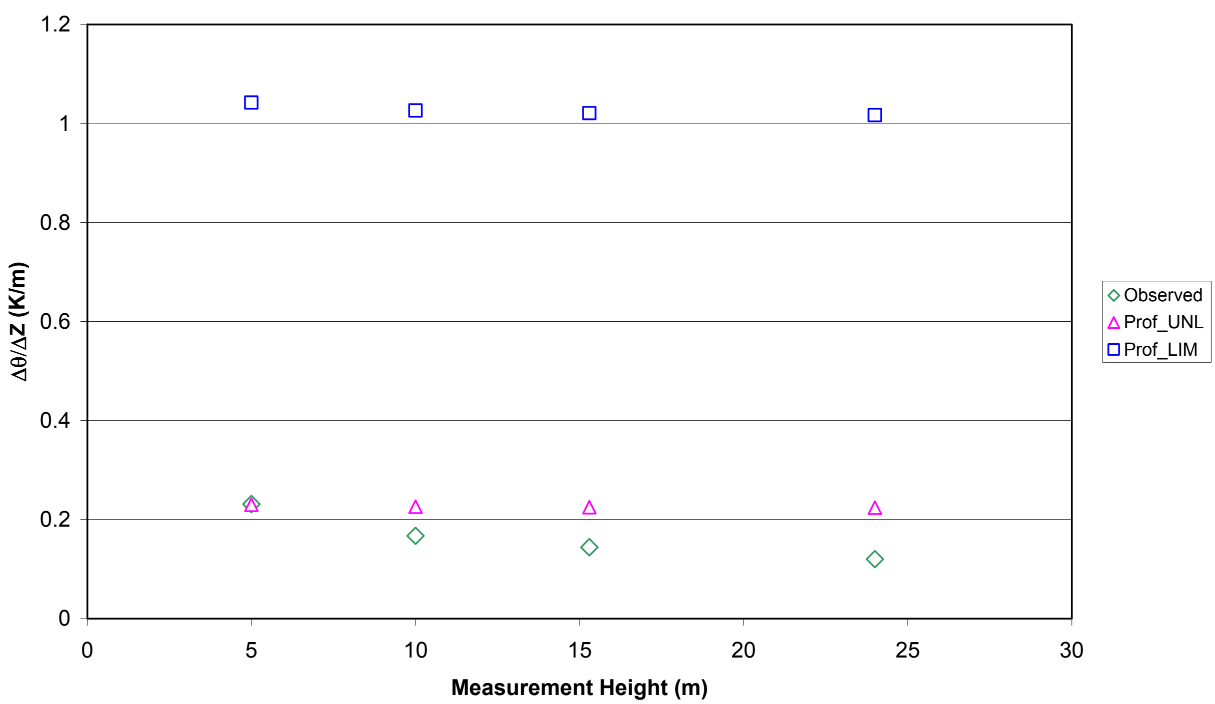

Figure 13. Comparison of Predicted to Observed Wind Speed for Prairie Grass

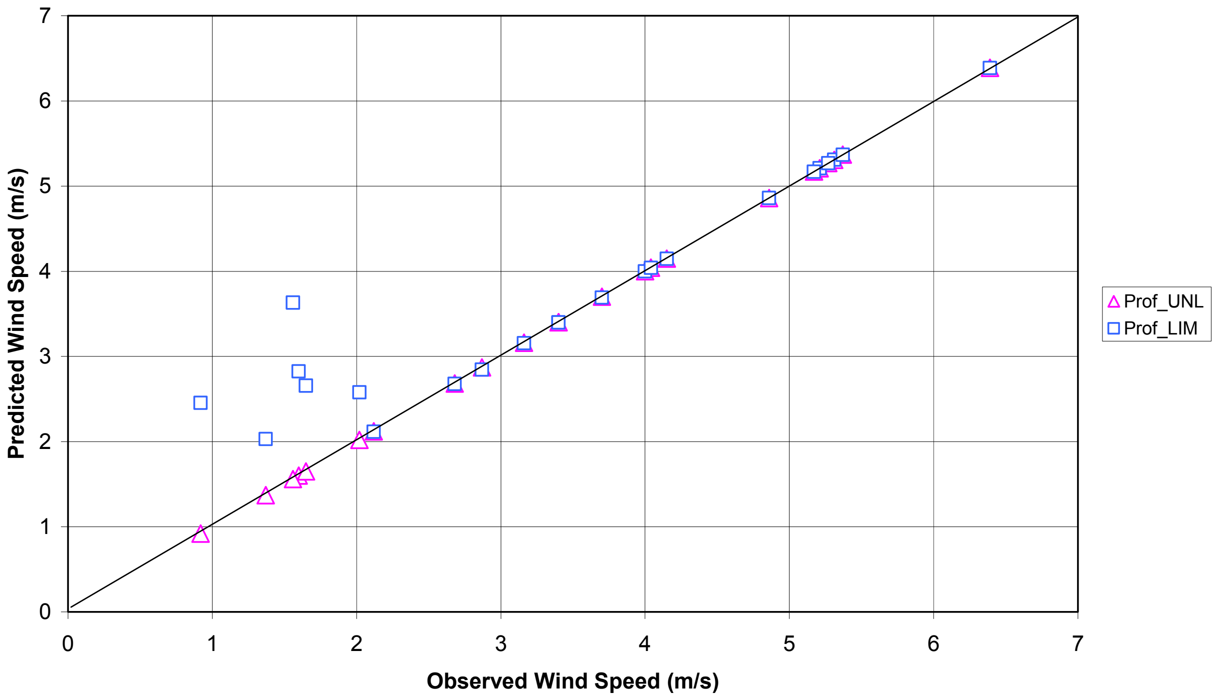

Figure 14. Comparison of Predicted to Observed ΔT for Prairie Grass

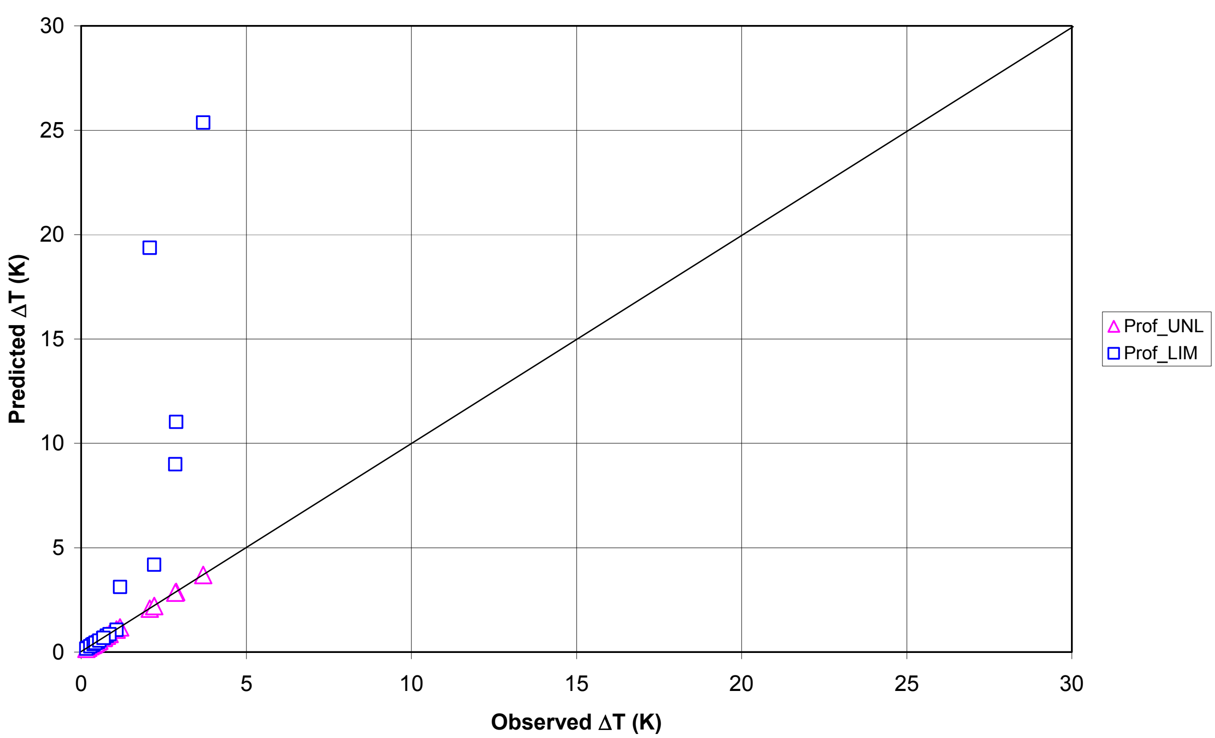

Figure 15. Observed vs. Predicted Wind Speed Profiles - Prairie Grass, July 22, Hour 20, Using WS@1m

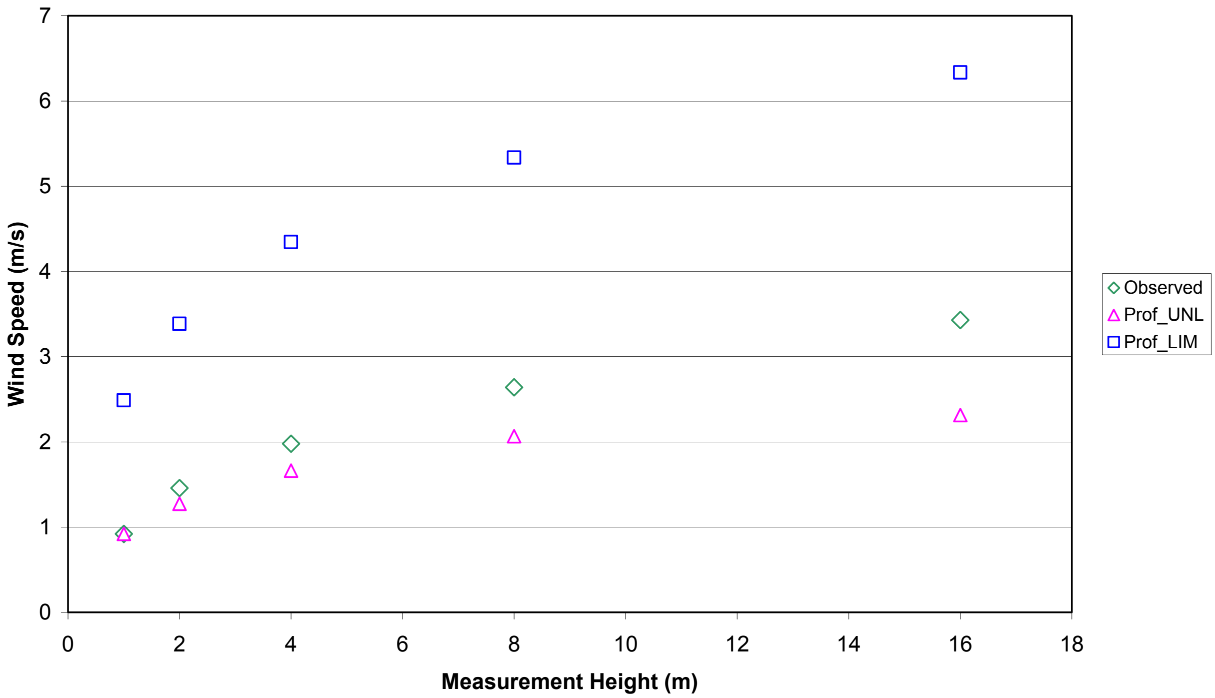

Figure 16. Observed vs. Predicted Δθ/ΔZ Profiles - Prairie Grass, July 22, Hour 20, Using WS@1m

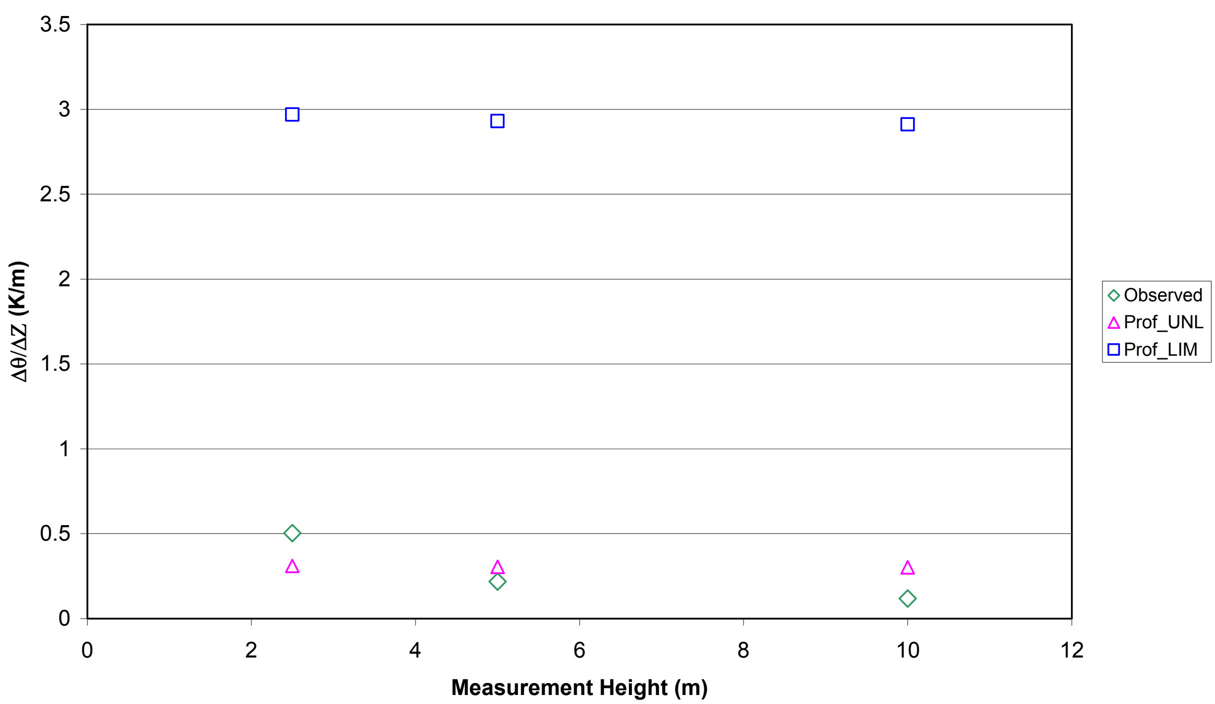

Figure 17. Observed vs. Predicted Wind Speed Profiles - Prairie Grass, July 22, Hour 20, Using WS@8m

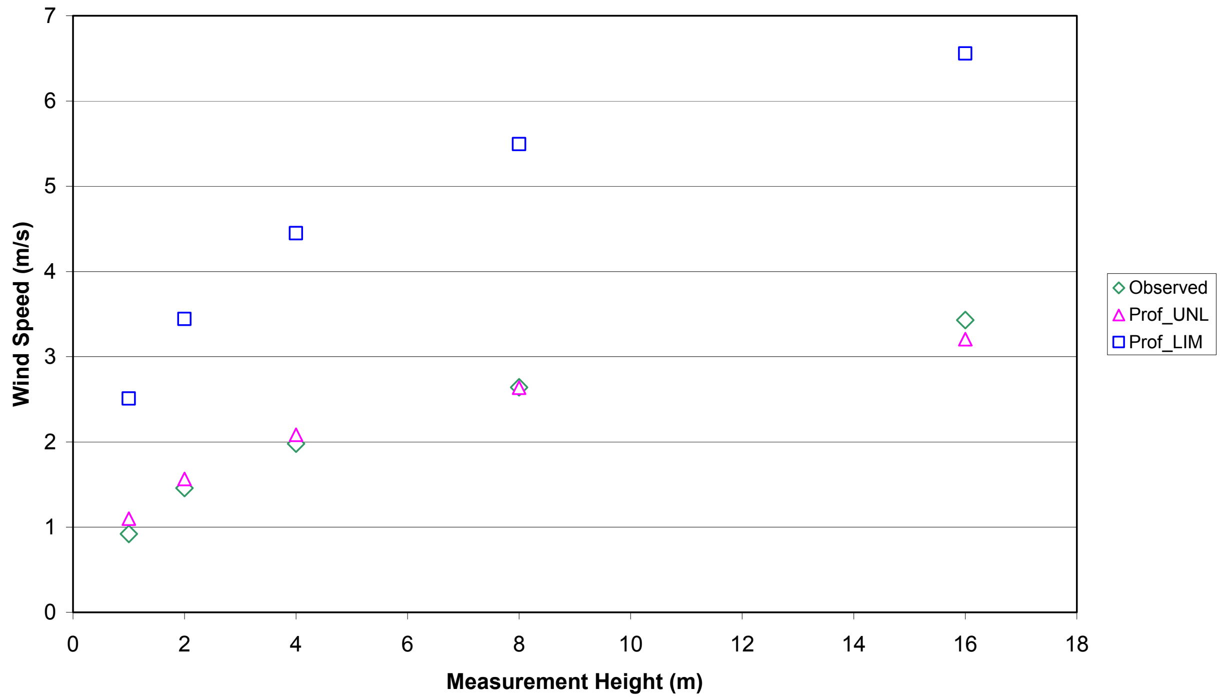

Figure 18. Prairie Grass 1-hr Q-Q Plot for SBL - BulkRi/Prof_UNL Method vs. CCVR

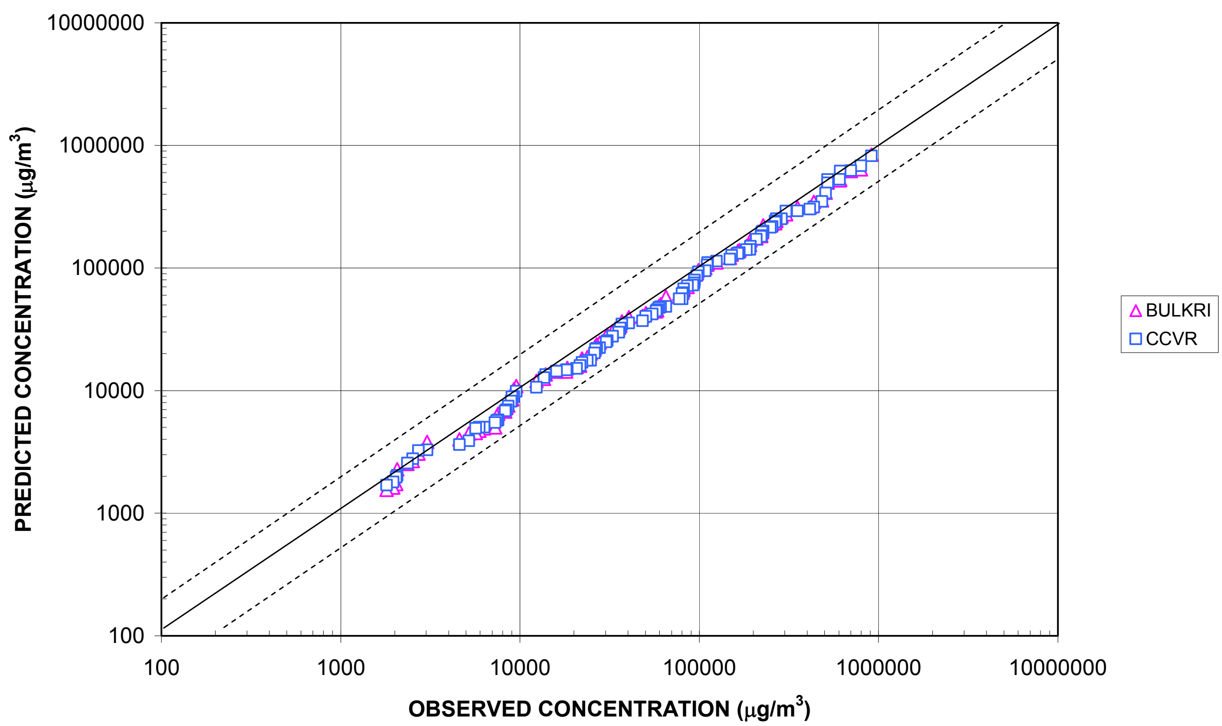

Figure 19. Prairie Grass 1-hr Q-Q Plot for SBL - BulkRi/02222 vs. CCVR

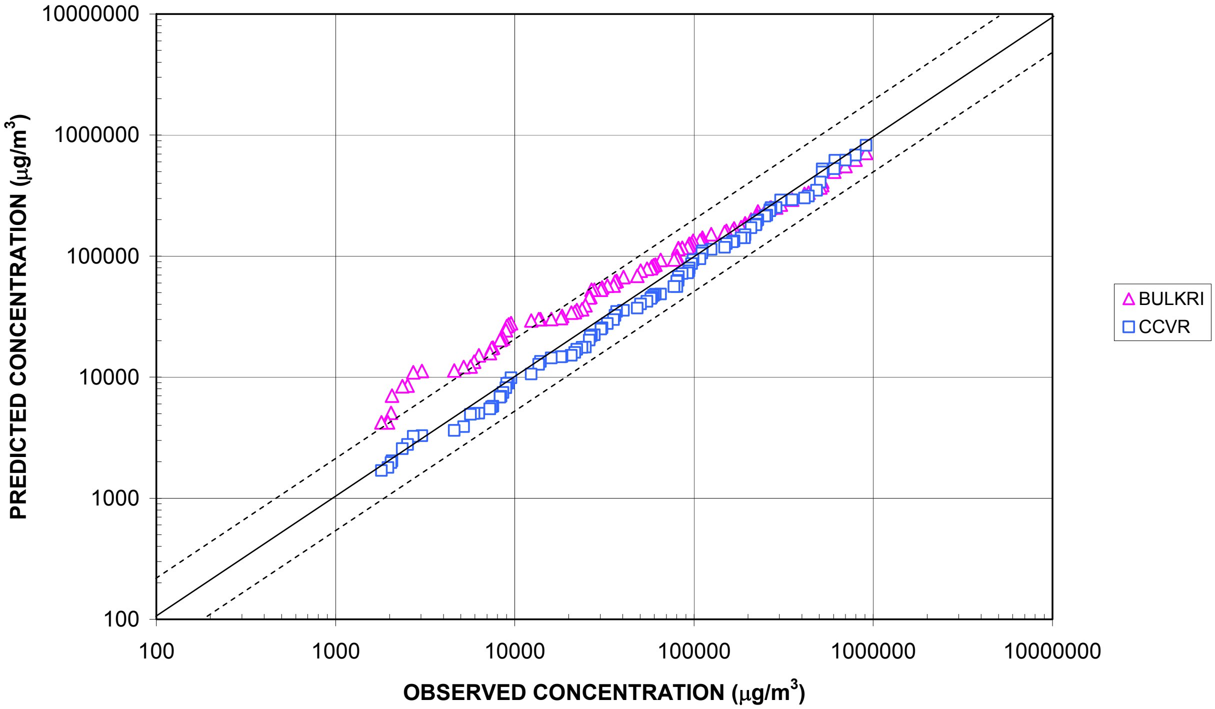

Figure 20. CCB SF6 χ/Qs - Hourly Maxima Q-Q Plot - BulkRi vs. CCVR

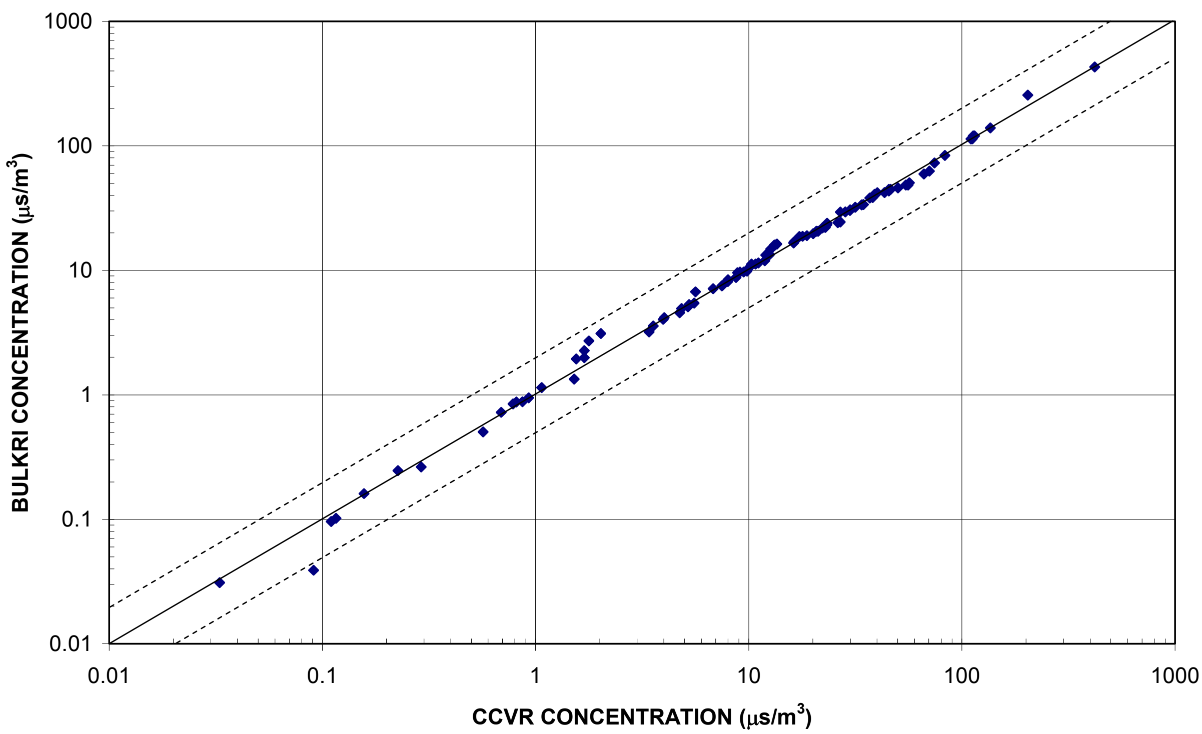

Figure 21. CCB SF6 χ/Qs - Hourly Maxima Paired in Time - BulkRi vs. CCVR

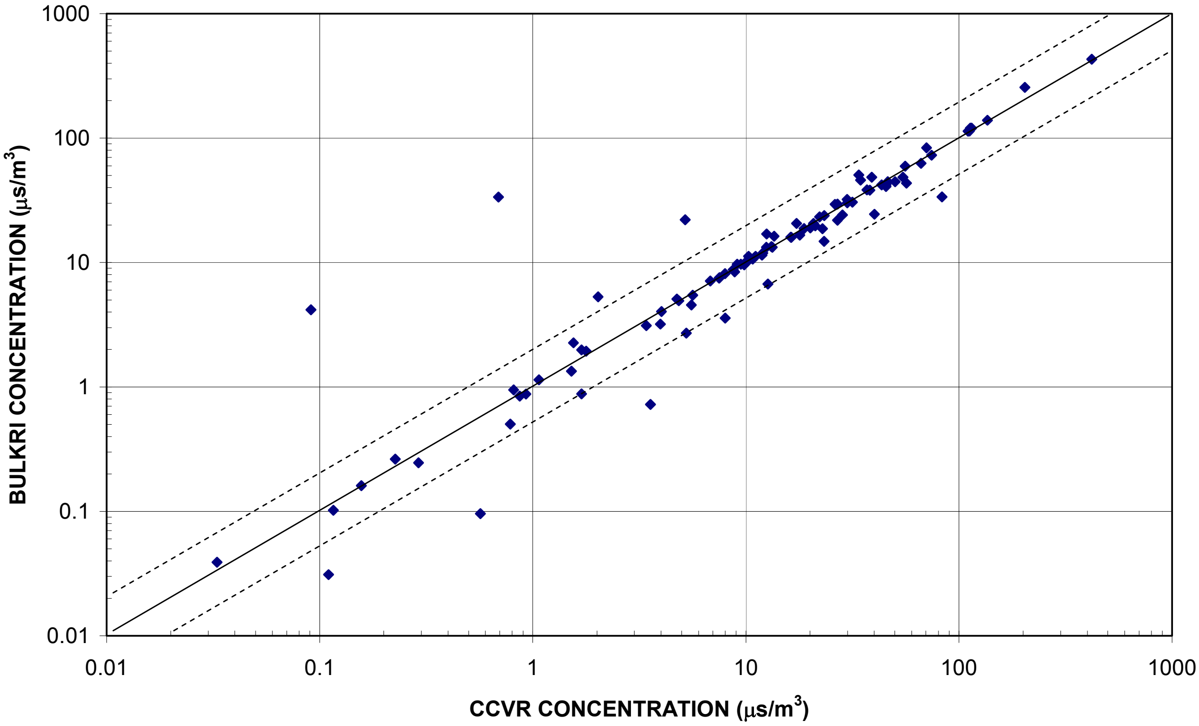

Figure 22. CCB SF6 1-Hr Q-Q Plot (χ/Q) - AERMOD/Prof_UNL Method vs. CTDM

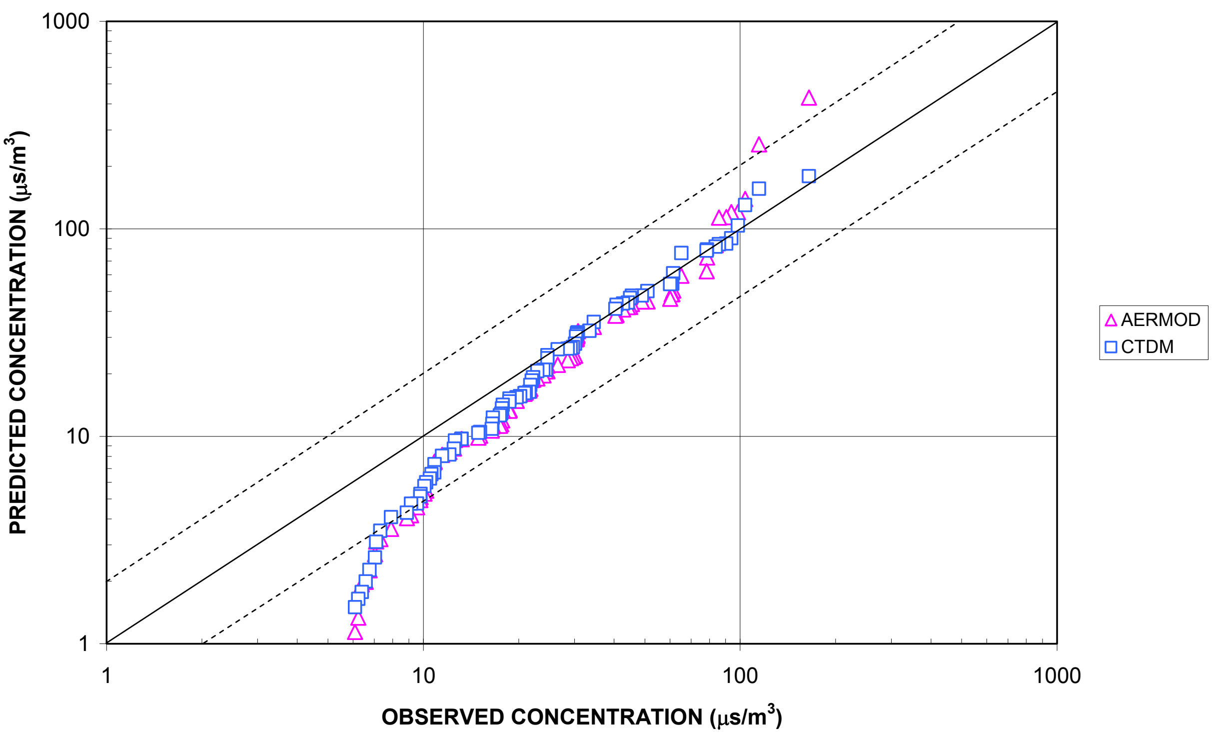

Figure 23. CCB SF6 1-Hr Q-Q Plot (χ/Q) - AERMOD/BulkRi/02222 vs. CTDM

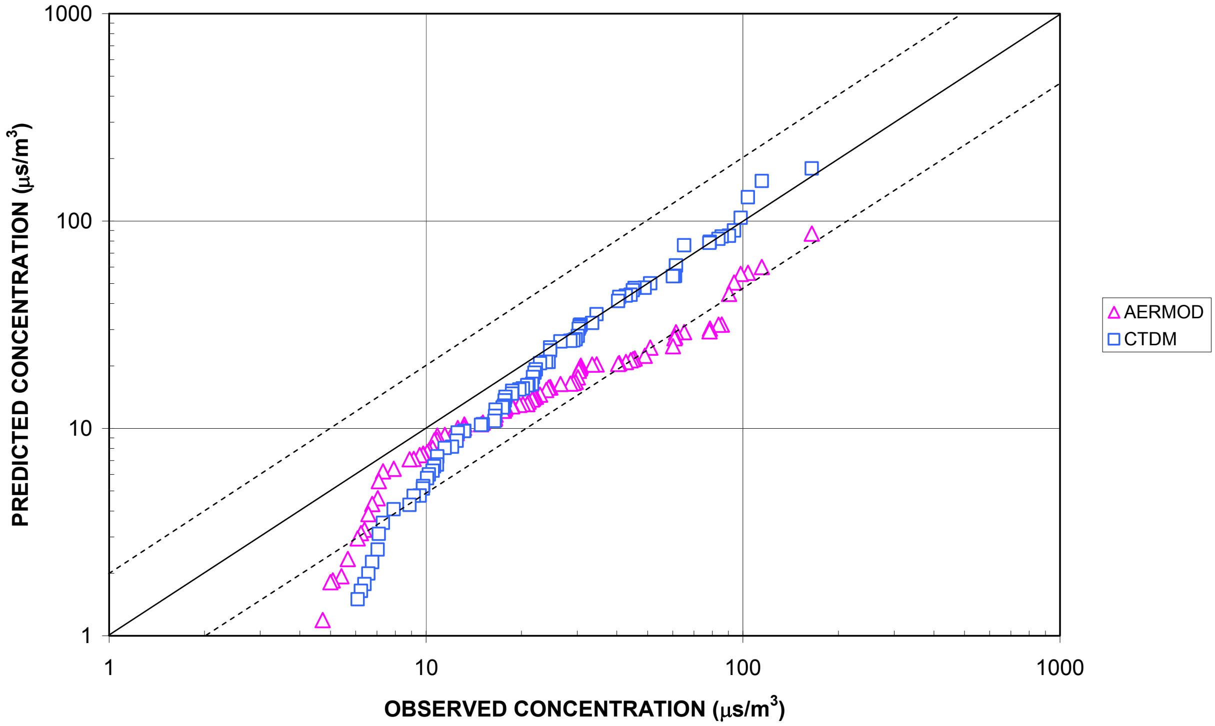

Figure 24. CCB SF6 1-Hr Q-Q Plot (χ/Q) - AERMOD/Prof_UNL vs. CTDM - No Sigma-w

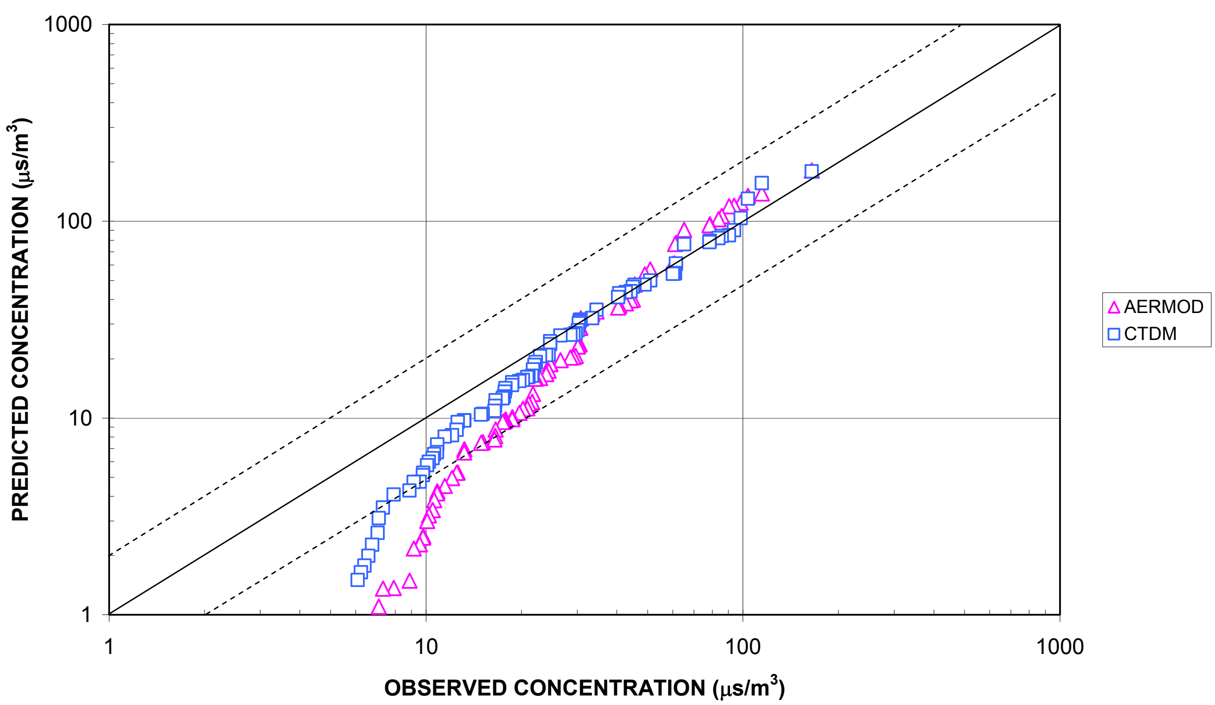

Figure 25. CCB SF6 1-Hr Q-Q Plot (χ/Q) - AERMOD/CCVR vs. CTDM - No Sigma-w