A comparison of CALPUFF air quality simulation results with monitoring data for Krakow Poland

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Keywords: Air Quality Modeling, Model Evaluation.

1 Introduction

The former Polish capitol, Krakow, is located in the valley of the Vistula river and frequently experiences extended periods of stagnation, especially in wintertime. With emissions from old technologies in the way of factories, steelworks, and small family manufactures, Krakow frequently experiences air pollution problems. In recent years, Krakow has seen a rapid increase in the numbers of cars and associated traffic congestion resulting from a lack of bypasses surrounding Krakow, which is anticipated to add to existing air pollution impacts. Starting in 1991 with support from the U.S. Environmental Protection Agency (EPA), a pilot program for Poland was initiated to develop a formal air pollution abatement program. A seven-station automated air-monitoring network was installed in Krakow and training was initiated in the collection and analysis of air monitoring data. In December 1998, the pilot program was extended to include training in the application of air dispersion modeling, for the ultimate purpose of investigating the benefits of alternative control abatement strategies. The CALMET/CALPUFF[1,2] modeling system was selected in order to provide a flexible system that would prove useful throughout Poland. In the following discussion we present preliminary comparisons of simulation results for sulfur-oxide (SO_2) with monitoring data for 1998.

2 Monitoring Locations and CALPUFF Model Setup

For 1998 there were 7 monitors in locations as shown in Figure 1. Site 1 was not in operation during June through August, but the other sites were in operation throughout the year. These monitors provide data for a variety of pollutants, but in this discussion we will focus on the hourly observations of SO_2.

The land use and terrain elevations were defined for a 100 by 100-km domain centered on Krakow using a grid resolution of 1-km, with Version 1.2 of the Earth Resources Observation Systems (EROS) data[3]. The U.S. Geological Survey land characterizations were used, but we found that the urban land use was limited and not representative of environs of Krakow. Therefore, we edited the files to define urban land use for all grids encompassed by the mobile source inventory, as illustrated in Figure 1.

Krakow airport provided hourly surface meteorological observations, and was approximately 10 km from monitoring Site 1. To provide coverage over the entire modeling domain, seven other meteorological sites were employed providing hourly surface meteorological observations, whose distance from monitoring Site 1 ranged from 67 to 137 km. Twice-daily upper air observations from four sites surrounding the modeling domain were available, but all were a considerable distance from Krakow, ranging from 119 to 300 km from monitoring Site 1.

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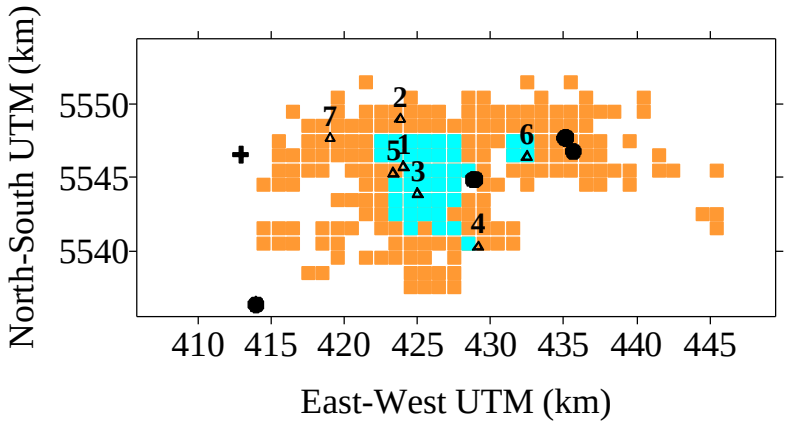

Figure 1 Illustration of original urban areas (blue squares), final urban areas (blue and tan squares), receptors (open triangles) and airport meteorological site (black plus sign). Solid circles are locations of major SO_2 point source emissions.

Results from a series of 10-day CALMET runs for January and June were inspected to check on the reasonableness of the meteorological fields being generated. Then 10-day simulations were performed with CALPUFF to check on the reasonableness of the dispersion characterizations. For the final runs, the dispersion parameters were computed internally using similarity theory with convective eddy effects modeled.

3 Emission Inventories

Emission inventories were constructed for mobile sources, heating emissions, and point sources for 1998. A mobile source emission inventory was constructed in an earlier study[4] providing annual average emission estimates for 1994 for 289 1-km grids. Based on an examination of traffic flow data, adjustments had been estimated for each month and time-of-day[4]. The mobile sources were treated as area sources with a 1-m release height and an initial vertical dispersion of 2.5-m. The inventories for heating and point source emissions were constructed for wintertime and summertime conditions. We used the summer inventories for the months May through August, and the winter inventories for the rest of the months. There were 321 1-km grids for the winter inventory and 266 1-km grids for the summer inventory. The heating emissions were specified as area sources with a release height and initial vertical dispersion equal to the average building heights in the grid. There were over 300 individual point sources, but most had annual SO_2 emission rates less than 10^{-3} g/s. We modeled the top 100 emitters as individual point sources, and grouped the rest of the point sources into 43 1-km grids for treatment as area sources. We later added six large sources all just outside of Krakow that had not been included in the original inventory. The four locations for six of the nine largest point sources for Krakow are shown in Figure 1 (solid black circles). Three point sources are outside of the area shown in Figure 1 (UTM coordinates 389, 5562), and together with the six sources depicted in Figure 1 account for over 95% of the point source SO_2 emissions. The emission characteristics for the nine largest point source, were reviewed and judged reasonable.

The mobile source and heat production emission inventories were considered preliminary. The mobile source inventory was constructed for 1994, and was judged to provide a reasonable spatial distribution of the emissions, but the magnitude of the emission rates (uncertain emission factors for polish mobile sources) was considered perhaps a factor of ten uncertain, depending on the pollutant being considered. The heat production emissions required emission factors and activity assumptions that were considered a factor of two uncertain, and no adjustments were provided to reflect an increase in heating emissions as ambient temperatures decrease. With these uncertainties, it was anticipated that some adjustments would be needed to tune the heat production and mobile source inventories for modeling.

The heating emissions are negligible during the summer. Thus it was decided to model June 1998 with the summer inventories, and determine a scaling factor for adjusting the mobile source emission rates by comparing the modeled and observed average SO_2 concentrations for the month

of June. Once the June analysis was completed, the winter months for 1998 would be modeled with the 'adjusted' mobile emissions, and a scaling factor would be determined for the heating inventory for each month, using a comparison of the average SO_2 concentrations modeled and observed for each month. Using this procedure, it was determined that the mobile emission rates needed to be scaled down by multiplying by 0.20. The monthly heating scaling factors were found to follow an expected progression in going from October through to April (0.1, 0.6, 1, 1, 1, 0.6, 0.1, respectively), reflecting an increase in emissions as ambient temperatures decrease. Given that the monitoring data have been used to adjust the emission rates for two of the inventories, we should judge the comparisons of modeled and observed concentration values to be presented with discretion.

4 Comparison of Modeling Results with Observations

The comparison of annual concentration values in Figure 2(A) suggest that emission inventories have been adjusted to a first order. The larger variance in the estimates versus that observed, may signal a need for 'local' emission inventory adjustments. For instance, the bias to overestimate concentration at Site 3, Figure 2(A), is seen in Figure 2(B) to relate to overestimation of the winter month concentration values (solid red circles). The bias to underestimate at Site 4, Figure 2(A), is seen in Figure 2(B) to relate to underestimation of the winter month concentration values (solid blue circles).

Figure 3 illustrates the estimated relative emissions for January and June 1998. Figure 4 illustrates the contribution to the total SO_2 concentration estimated for Site 5 from each of the three emission inventories. Only results for Site 5 are shown in Figure 4 since the contribution from the three emission inventories (point, heat, mobile) to the total SO_2 concentration estimated at each site is fairly consistent across all sites. Figure 4 shows the definite seasonal variation in the relative impact from the three source types, and the relative importance during the heating season of the heat production emissions. These results shown in Figures 3 and 4 illustrate that although the emissions from tall stacks can be considerably larger than from low level releases, the local impact from these emissions is limited to periods of the day and seasons of the year when these emissions reach the surface.

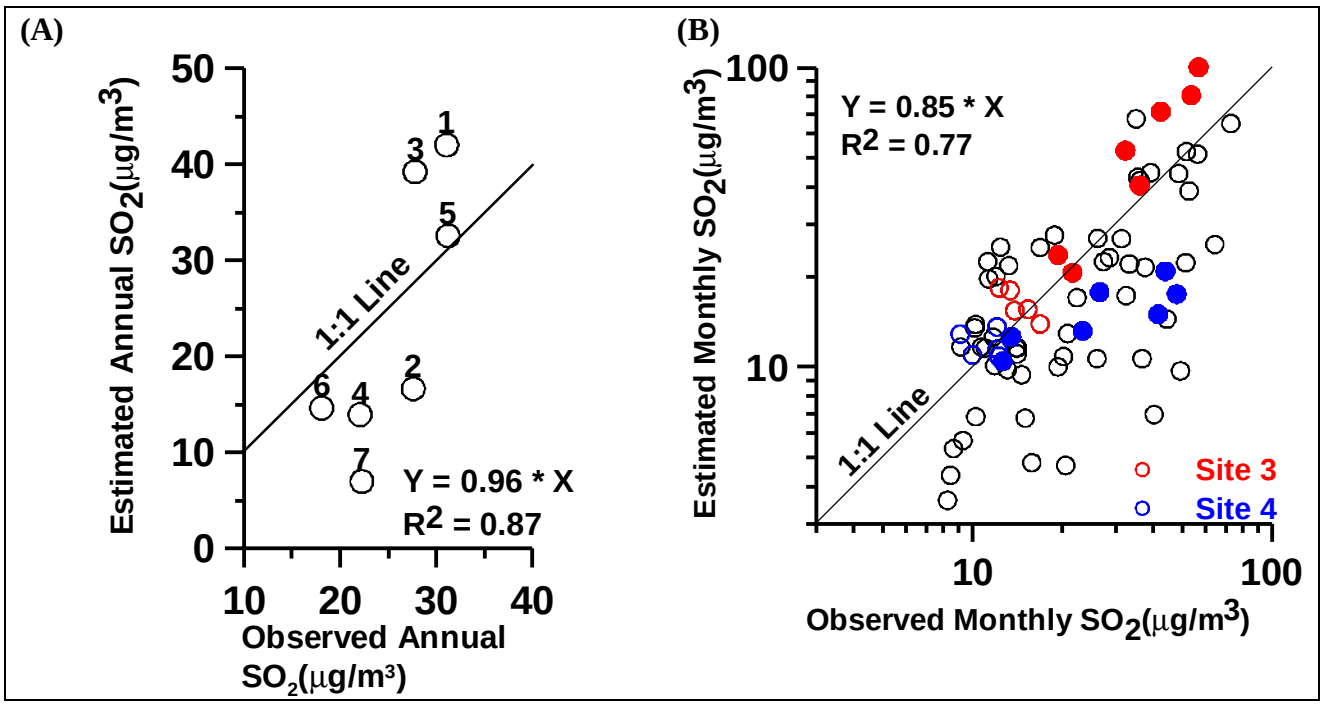

Figure 2 Comparison of observed and estimated A) annual average and B) monthly average SO_2 concentration values. Linear regression results (with zero intercept) and site locations are annotated within the figures.

To further compare the model estimates with the observations, the estimated and observed time series of hourly concentration values were decomposed using the Kolmogorov–Zurbenko (KZ) filtering technique[5,6]. The time series were separated into four scales representing intra-day, diurnal, synoptic, and baseline, using 3 KZ filters: KZ(3,3), KZ(13,5) and KZ(103,5). The notation[5,6] KZ(13,5) indicates use of a 13 hour running average that is applied 5 times.

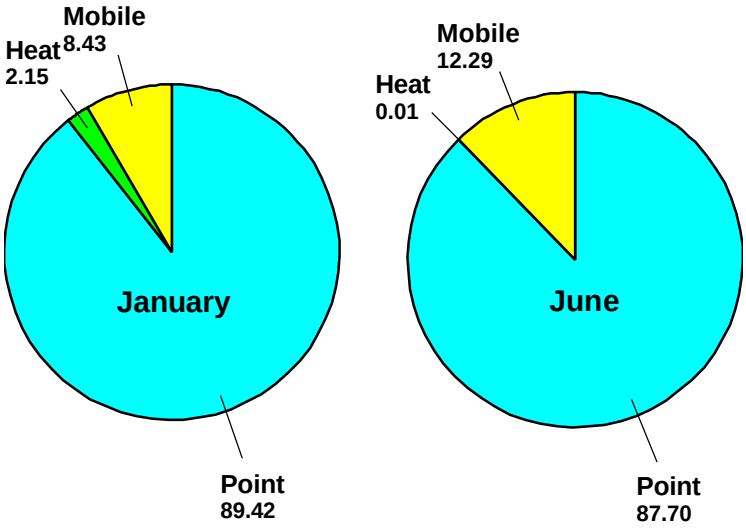

Figure 3 Relative emissions (percent) for January and June

Figure 5 depicts the baseline results for Sites 3-5, and the intra-day, diurnal and synoptic scales for Site 5. The baseline comparisons suggest that the model is tracking the seasonal and certain weekly events well, as can be seen in the correspondence of the baseline patterns around the end of March (sequential hour 2000). There is a general trend to overestimate concentrations across all sites in August and September (sequential hours 5000 through 7000). The KZ time series for the other scales have a zero mean, and the main comparison point is whether the observed and estimated variances are similar. As can be seen in Figure 5(B), which is illustrative for all the sites, the modeled time series has a larger variance at all time scales than is seen in the observations.

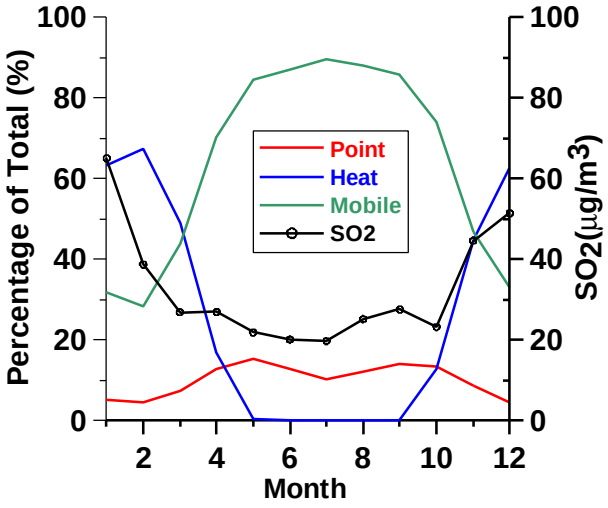

Figure 4 The percentage contribution to the total SO_2 concentration estimated for Site 5 from each of the three emission inventories. Black line is simulated total SO_2.

6 Conclusions

Scaling factors were determined and applied for varying the heat production emissions throughout the heating season, and scaling the mobile emissions to provide better correspondence with observations. The modeled concentration values appear to track specific events in the baseline time series. There are periods (particularly in August and September) needing further study. In the simulations presented, the background SO_2 concentration was assumed to be zero. While this seems to be generally true, the large industrial SO_2 emissions from Katowice (80 km west of Krakow), likely play an important role during certain synoptic conditions which warrants further consideration. The variance of the estimated intra-day, diurnal and synoptic KZ time series is often twice that seen in the observations. It is speculated that mixing induced by buildings and structures 'diffuses' the individual emissions, whereas the modeled time series retains the specific 'signatures'

of the individual source plumes. Thus, the modeled time series reflects the spikes of individual plumes as they hit and miss the receptors.

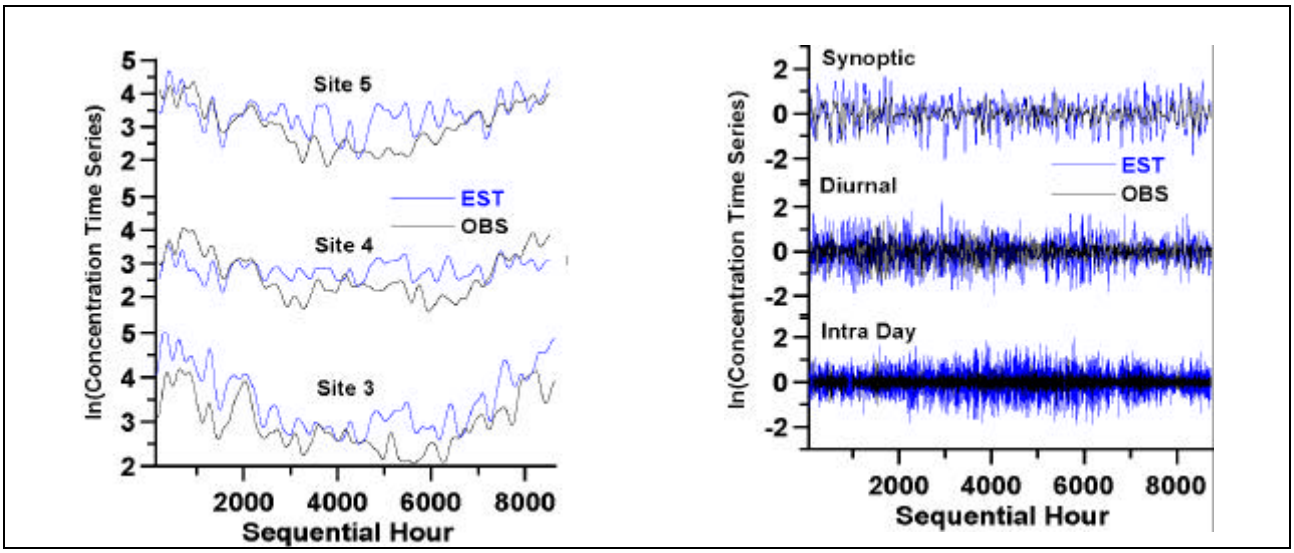

Figure 5 KZ filter results depicting the (A) baseline time series for three site, and (B) intra day, diurnal and synoptic time series for Site 5.

Disclaimer

This work was funded in part by the United States Environmental Protection Agency through an Interagency Agreement (DW 13937039-01-06) with the National Oceanic and Atmospheric Administration. It currently is being subjected to Agency review for approval for publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

References

1. Scire, J.S., Yamartino, R.J., and Fernau, M.E., (2000a): A user's guide for the CALMET meteorological model. Earth Tech, Concord, MA., http:\\www.src.com (accessed March, 2000).
2. Scire. J.S., Strimaitis, and Yamartino, R.J., (2000b): A user's guide for the CALPUFF dispersion model. Earth Tech, Concord, MA., http:\\www.src.com (accessed March, 2000).
3. Data is available at this web site. http://edcdaac.usgs.gov/glcc/glcc.html
4. Oszacowanie Zanieczyszczen Komunikacyjnych Na Terenie Miasta Krakowa, Computer Service Poland, 30-233 Krakow, ul. Berberysowa 18, 1996, 296 pages.
5. Eskridge, R.E., Ku, J.Y., Rao, S.T., Porter,P.S., Zurbenko, I.G., (1997): Separating Different Scales of Motion in Time Series of Meteorological Variables. *Bulletin of the American Meteorological Society*, Vol. 78, (7):1473–1483.
6. Rao, S. T., Zurbenko, I.G., Neagu, R., Porter, P.S., Ku, J.Y., Henry, R.F., (1997): Space and Time Scales in Ambient Ozone Data. *Bulletin of the American Meteorological Socie*ty, Vol. 78, (10):2153–2166.