Results
GC-MS Calibration Samples
Three direct injection calibration samples, which contained all but one of the training set compounds, were analyzed [2]. Of the 77 compounds observed in the calibration runs, 84% were correctly identified. Of the 13 compounds not identified, three were correctly assigned by chemical class.

GC-MS Field Samples
The GC-MS data files for three field samples were also analyzed [3]. The identities of the target compounds were determined by using both GC retention times and a combination of forward and reverse spectral matching techniques with stringent matching parameters. The identification of other compounds not on the target list was based on a Finnigan search technique. The application of the pattern recognition scheme to the transformed data for the target compounds resulted in 88% correct classification. The compound identification results were 85% accurate.

There were 75 different nontarget compounds identified in 120 occurrences in the three samples. The classification results agreed very well for the two class I and class 2 spectra. However, a very large number of alkanes and alkenes were incorrectly classified as chlorocompounds. Further details of this study are given in references [2], [3], and [4].

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References

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coated with Teflon. The impactor surface is a sintered glass disc coated with silicone grease to prevent particle bounce. At 16.7 L/min, a 50% D_{AB} = 2.64 \mu m cutpoint was obtained with an impactor nozzle jet diameter of 4.0 mm (Baxter and Lane [2]).

The first two denuder tubes were coated with a 1% solution of glycerine and Na_{2}CO_{3}. Anions collected on the second denuder are used to correct for any particle deposition that may have occurred in the denuders during sampling. Both denuders were extracted with ion chromatography eluent and analyzed for NO_{3}^{-}, NO_{2}^{-}, N\text{O}_{3}, (HNO_{3}), and (SO_{2}). The two filters in the filter pack were extracted with 20 mL deionized water and analyzed for SO_{4}^{-} and NO_{3}^{-} content. For some portions of the study, a third annular denuder coated with citric acid was used to collect NH_{3}. As a result of these experiments, we have demonstrated that a relatively inexpensive ($150.00) Teflon-coated impactor will quantitatively transmit acidic gases to an annular denuder.

In addition, modifications to the annular denuder itself resulted in a reliable system for field investigations. Paired samples were run to compare the new denuder assemblies and the average percent differences between sampler results with different inlet configurations for SO_{2}, HNO_{3}, HNO_{2}. The differences were 3.4, 6.4, and 8.3%, respectively. During the second phase of the testing, an NH_{3} denuder was incorporated into the assembly. The average % difference between two identical annular denuder systems for SO_{2}, HNO_{3}, HNO_{2}, NH_{3}, SO_{4}²⁻ and NO_{3}⁻ were 1.8, 5.5, 15, 16, 4.6 and 3.6%, respectively. Experiments by Appel et al. [3] indicated that HNO_{3} was not retained in the Teflon-coated glass inlets.

In our study, intercomparison of denuder assemblies showed that ratios of HNO_{3} to particle nitrate tended to decrease with decreasing ambient temperature and increasing humidity. This is qualitatively consistent with previous theoretical phase equilibrium calculations of NH_{4}NO_{3}.

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