

Introduction to the Xact 625i Ambient Metals Monitor



Presentation Outline

- Operation and Capabilities of the Xact 625i
- Comparison Studies
- How researchers are using the data in source identification and apportionment

Difficulties of Traditional Metals Monitoring



- 24 hour integrated sample
- Laboratory analysis – results in 4 to 6 weeks – **SLOW**
- Very little time resolution and no diurnal variability information
- Labor Intensive – field labor gathering the samples and analysis in the laboratory (usually using XRF, ICP-MS, ICP-OES)
- Takes a long time to get a data set that can provide good statistics for source apportionment

Advantages of Near Real Time Monitors



- Provides near real time metals concentration data – with time resolution as low as 5 minutes (most users are 1 hour)
- Uses reel to reel filter tape (similar to BAM) followed by analysis by energy dispersive X-ray Fluorescence (XRF)
- Xact 625i is able to measure up to 67 different elements simultaneously (44 is standard configuration)
- Little user interaction required
- Can get a statistically meaningful data set in a shorter period of time
- Can observe diurnal variability and other time dependent trends

Elements Measurable

H																	He	
Li	Be											B	C	N	O	F	Ne	
Na	Mg											Al	Si	P	S	Cl	Ar	
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	**	Rf	Ha	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo	
		* Lanthanide Series		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
		** Actinide Series		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

- Xact 625i can measure all elements in blue
- Xact can measure up to 67 elements simultaneously
- Standard Configuration includes 44 elements

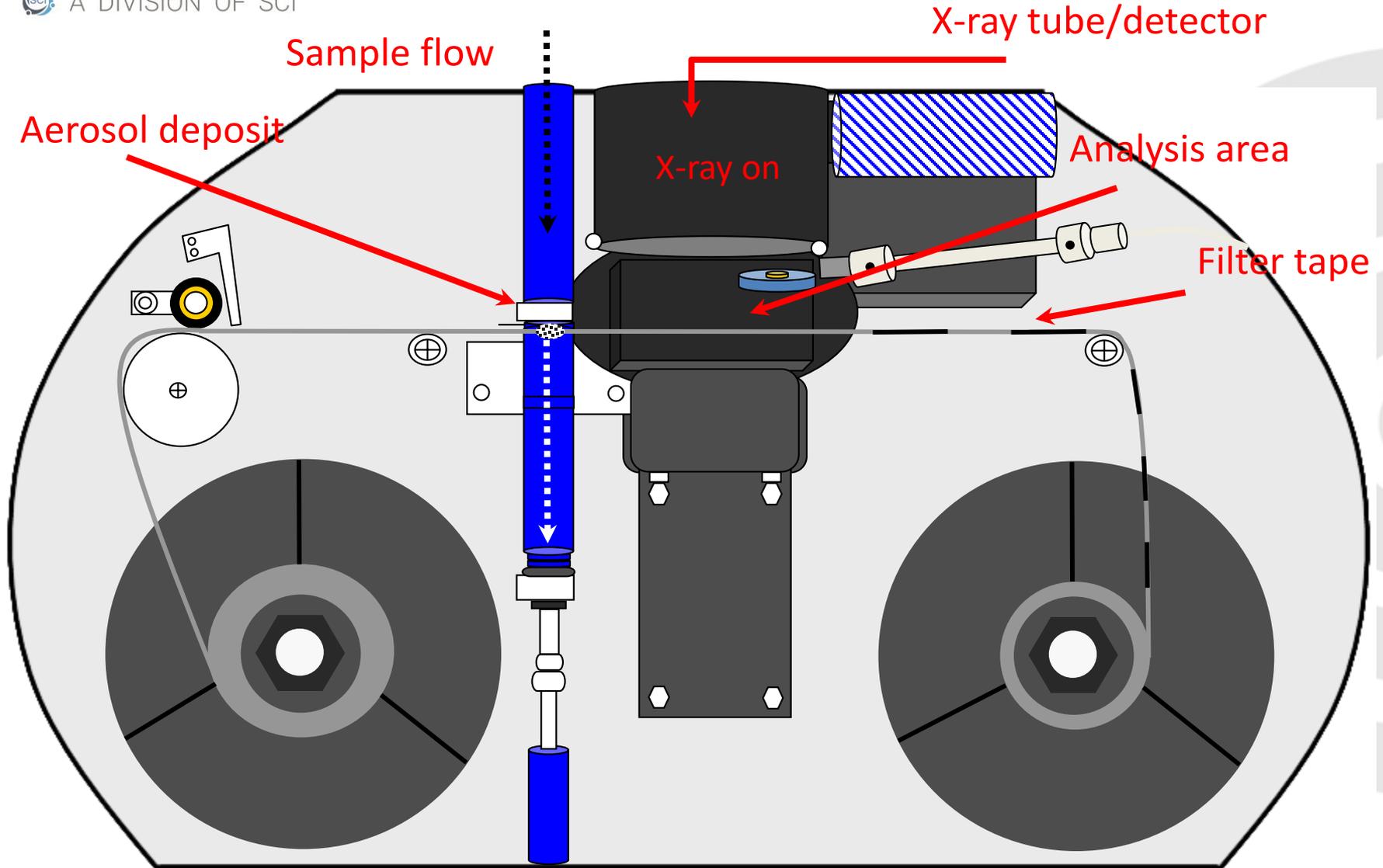
Detection Limits

Xact 625i Minimum Detection Limits (ng/m³)
68% Confidence Level (C1σ) per US EPA IO 3.3 and Currie *

Element	Atomic Number	15	30	60	120	180	240
		Al	13	840	290	100	35
Si	14	150	51	17.8	6.3	3.4	2.2
P	15	44	15	5.2	1.8	0.99	0.64
S	16	26	9.1	3.16	1.1	0.60	0.39
Cl	17	15	5.0	1.73	0.61	0.33	0.21
K	19	9.8	3.4	1.17	0.41	0.22	0.14
Ca	20	2.5	0.86	0.30	0.10	0.057	0.037
Ti	22	1.3	0.46	0.16	0.056	0.030	0.020
V	23	1.0	0.34	0.12	0.042	0.023	0.015
Cr	24	0.97	0.33	0.12	0.041	0.022	0.014
Mn	25	1.2	0.41	0.14	0.050	0.027	0.018
Fe	26	1.4	0.49	0.17	0.061	0.033	0.021
Co	27	1.1	0.39	0.14	0.049	0.026	0.017
Ni	28	0.78	0.27	0.10	0.034	0.018	0.012
Cu	29	0.65	0.23	0.079	0.028	0.015	0.010
Zn	30	0.55	0.19	0.067	0.023	0.013	0.008
As	33	0.52	0.18	0.063	0.022	0.012	0.008
Se	34	0.66	0.23	0.081	0.029	0.016	0.010
Br	35	0.85	0.30	0.10	0.037	0.020	0.013
Ag	47	16	5.5	1.9	0.68	0.37	0.24
Cd	48	21	7.2	2.5	0.89	0.48	0.31
In	49	26	8.9	3.1	1.1	0.60	0.39
Sn	50	33	12	4.1	1.4	0.78	0.51
Sb	51	42	15	5.2	1.8	0.99	0.64
Ba	56	3.3	1.1	0.39	0.14	0.074	0.048
Hg	80	0.99	0.35	0.12	0.043	0.023	0.015
Tl	81	0.95	0.33	0.12	0.041	0.022	0.014
Pb	82	1.0	0.36	0.13	0.045	0.024	0.016
Bi	83	1.1	0.37	0.13	0.046	0.025	0.016

- Detection limits are similar to those achieved using laboratory analysis
- Detection limits are under 1 nanogram for most trace elements
- Detection limits depend on sampling and analysis time
- Trade offs between the importance of time resolution and detection limit

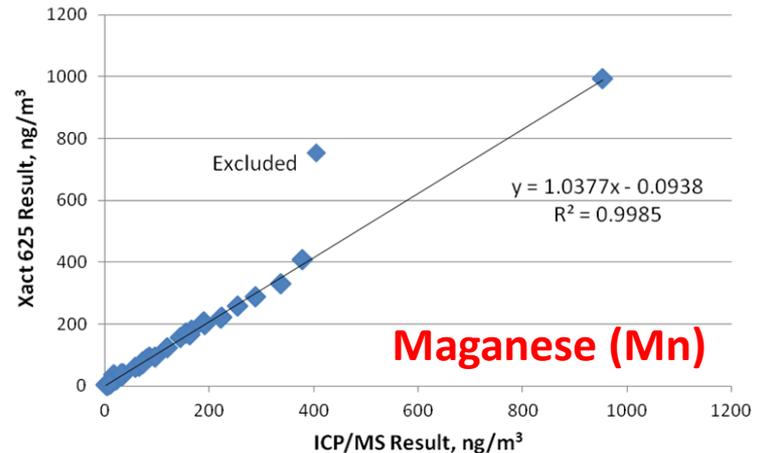
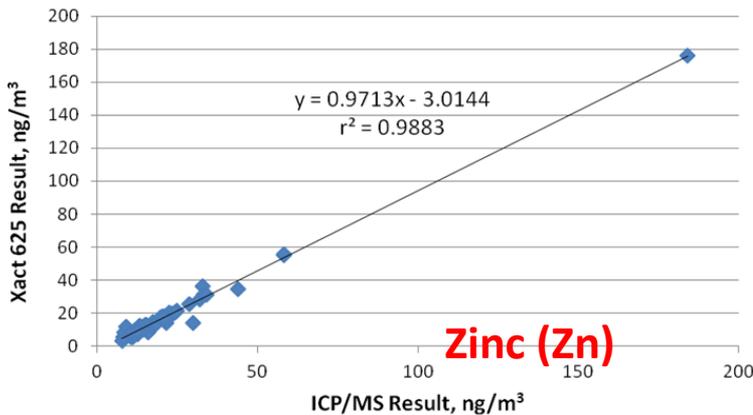
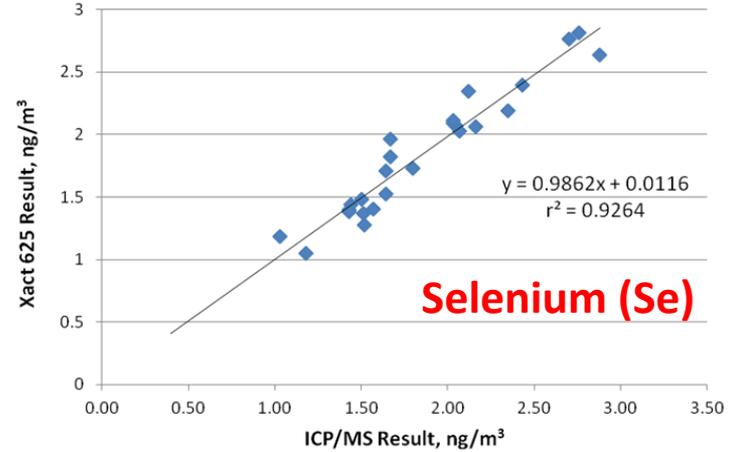
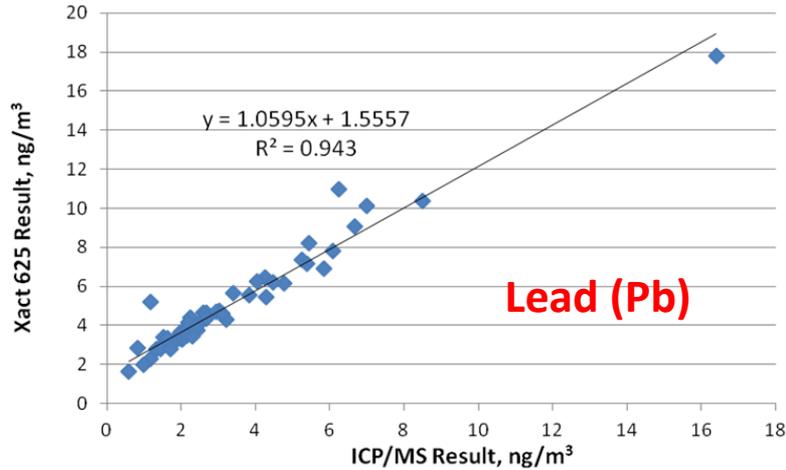
Internal Operation



Comparison Studies

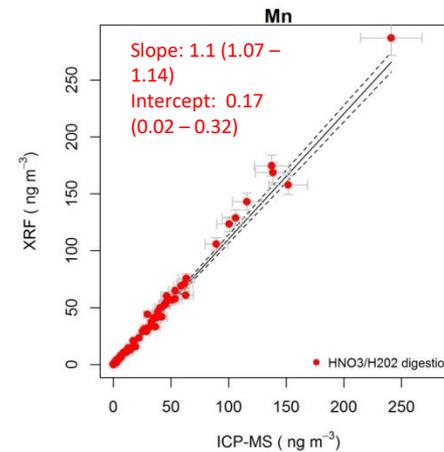
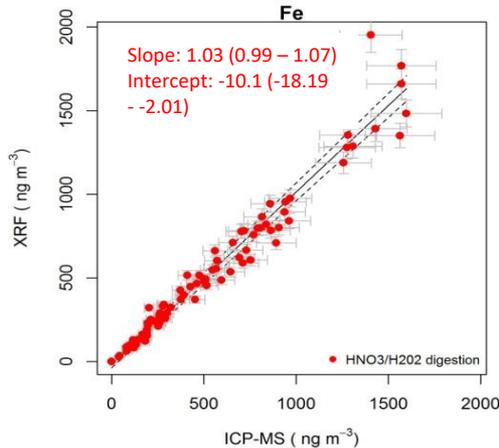
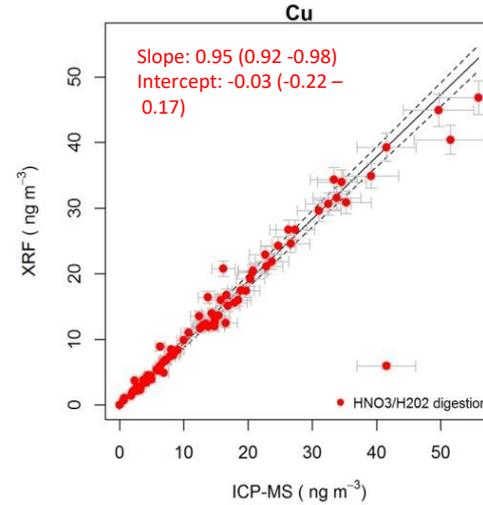
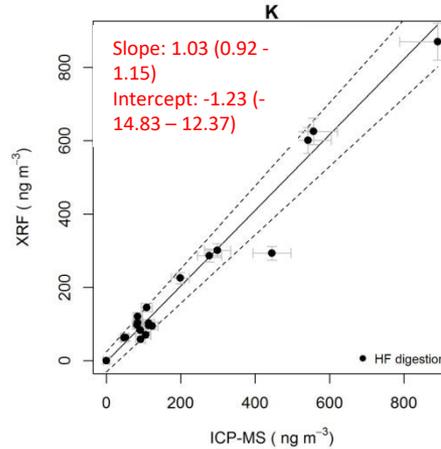
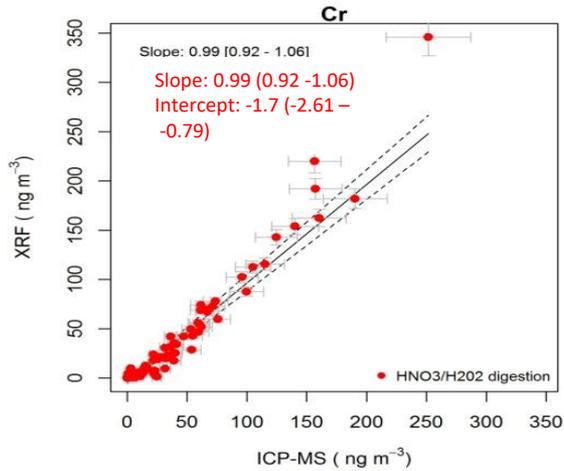
- Comparison studies are important so that you know the quality of the data used in your source identification/apportionment study
- Comparison studies reviewed all involve the Xact
 - US Environmental Protection Agency Environmental Technology Verification (ETV)
 - Study by King's College London

Comparison Studies-US EPA ETV

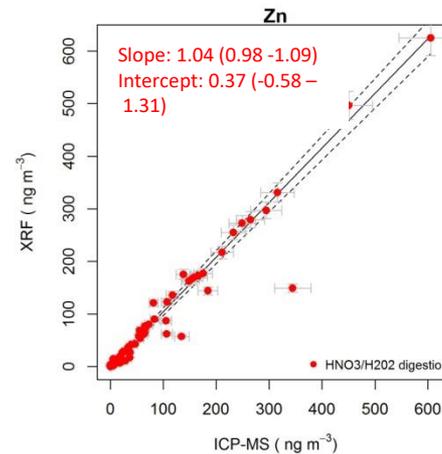
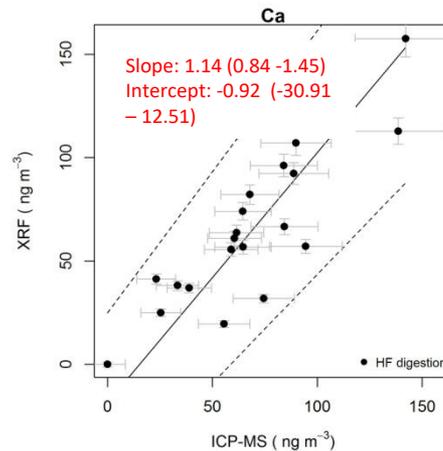
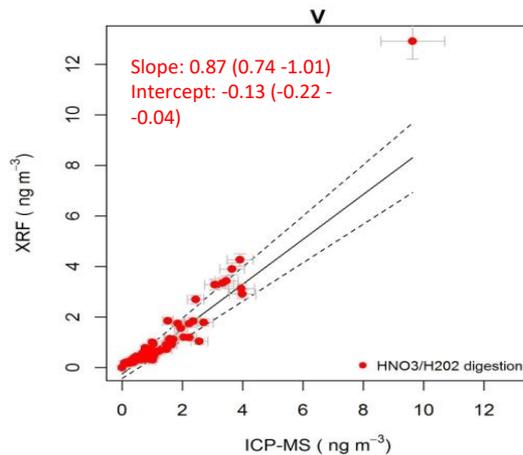
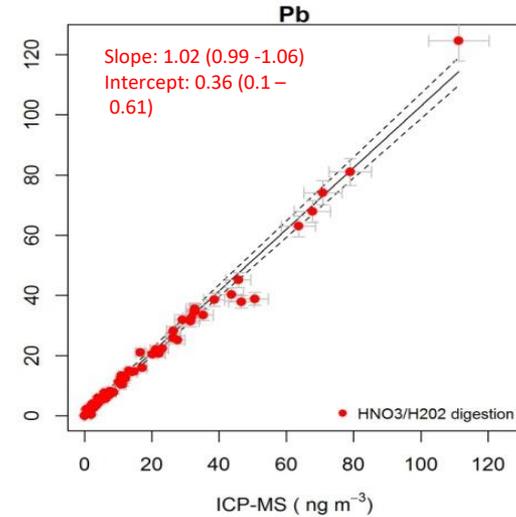
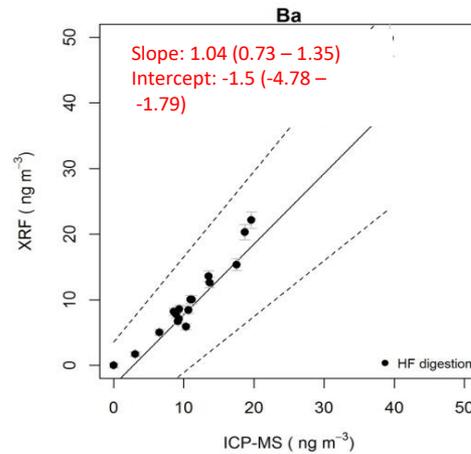
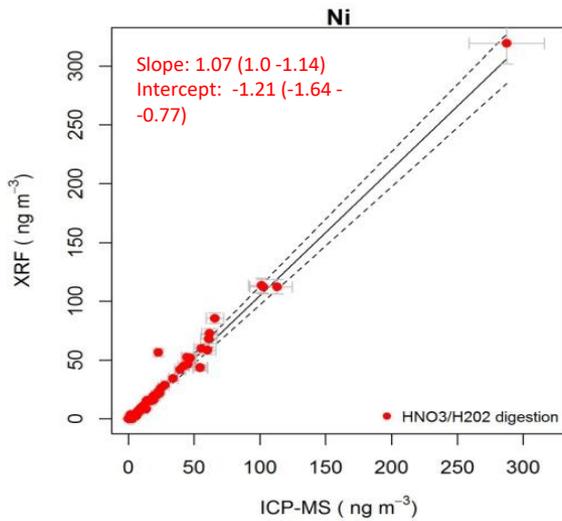


- Slopes are close to one indicating good agreement between Xact and Laboratory ICP-MS
- High Correlation Coefficient indicates good precision

Comparison Studies – King’s College London



Comparison Studies – King’s College London



Approaches to Source Identification and Apportionment Using the Xact 625i

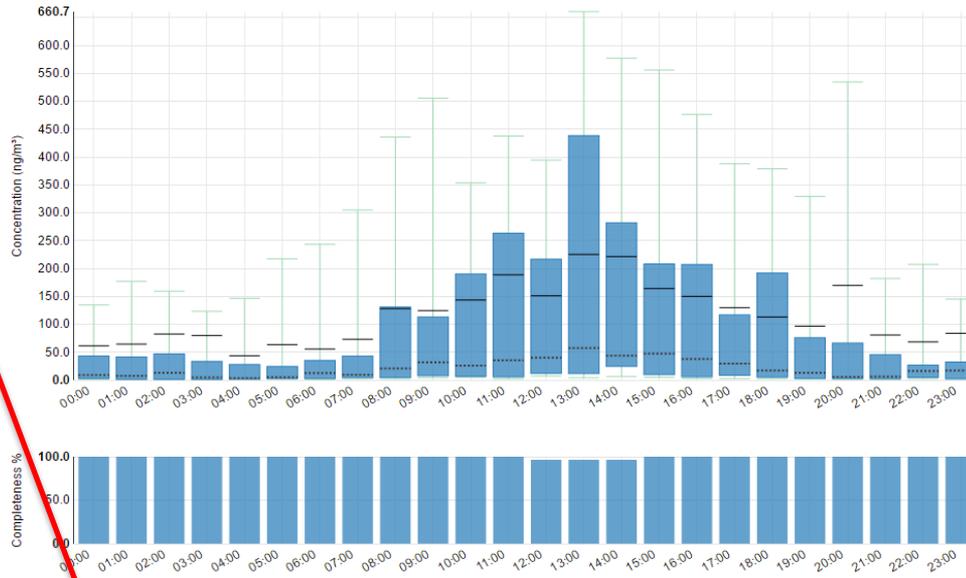
- Direct Data Approach – Using concentration data and meteorological data
- Network Data Approaches
- Source Apportionment – PMF, PCA
- Time resolved size fraction partitioning
- Localized plume identification with ultra high time resolution data

Direct Data Approaches – Time of Day



Elemental Metals

- Ti Titanium
- V Vanadium
- Cr Chromium
- Mn Manganese
- Fe Iron
- Co Cobalt
- **Ni Nickel**
- Cu Copper
- Zn Zinc
- As Arsenic
- Se Selenium
- Rb Rubidium
- Sr Strontium
- Mo Molybdenum
- Cd Cadmium
- Sn Tin
- Sb Antimony
- Ba Barium
- Pt Platinum
- Hg Mercury
- Pb Lead



- This plot shows a nickel source that is present during the day
- Xact comes with software package to automatically generate these plots

- Metals can fluctuate widely over the course of a day
- Box and whisker shows concentration variability with time of day
- Provides information about when a source is contributing

Direct Data Approaches – Correlation Between Measured Elements



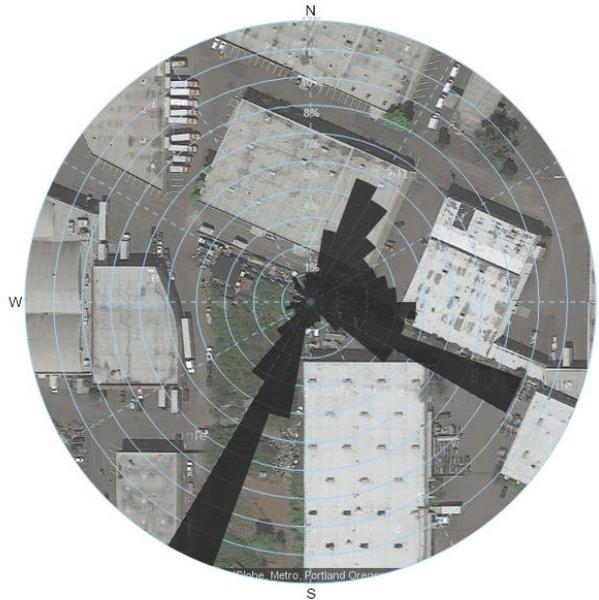
- Shows plot of every element versus vanadium
- Correlation Coefficients are displayed on the plot
- Elements that are highly correlated are likely from the same source – e.g. Ni, Co and Mo

Direct Data Approaches – Correlation with Wind Direction



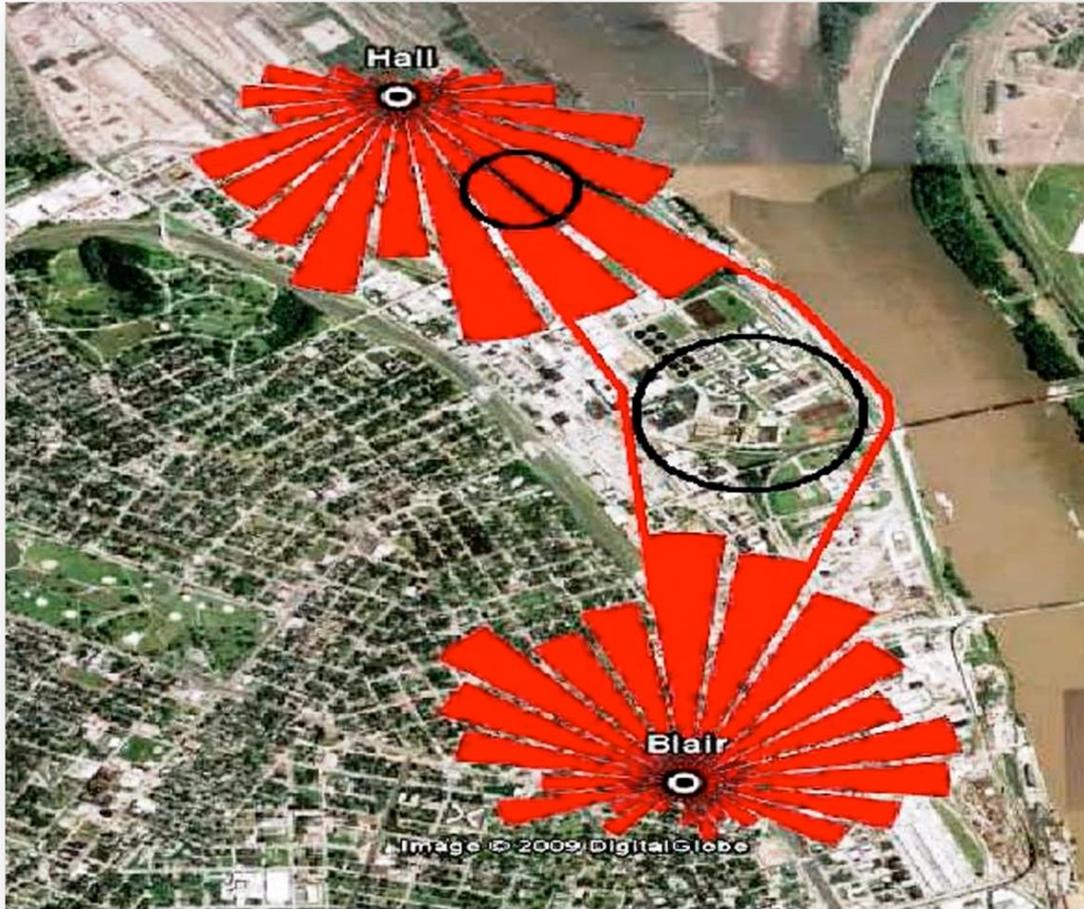
Elemental Metals

- Ti** Titanium
- V** Vanadium
- Cr** Chromium
- Mn** Manganese
- Fe** Iron
- Co** Cobalt
- Ni** Nickel
- Cu** Copper
- Zn** Zinc
- As** Arsenic
- Se** Selenium
- Rb** Rubidium
- Sr** Strontium
- Mo** Molybdenum
- Cd** Cadmium
- Sn** Tin
- Sb** Antimony
- Ba** Barium
- Pt** Platinum
- Hg** Mercury
- Pb** Lead



- Plot shows the directionality of highest concentrations (75th percentile)
- Locate sources by correlating high concentration events with wind direction

Direct Data Approaches - Triangulation



- Correlate data from multiple instruments at multiple locations with wind direction
- Use the resulting pollution rose to identify location of source

Source Apportionment

- Xact 625 data has been involved in many peer reviewed source apportionment studies over the last few years
 - Source apportionment of total PM_{2.5} or PM₁₀ – data used in conjunction with other measurements
 - Although metals constitute a small percentage of total PM – they are key tracers in identifying sources
 - Source apportionment of total measured metals
 - Since metals are often highly reactive they can have an outsized influence on air pollution health effects
 - Therefore identification of metals sources can be important in its own right
- Higher time resolution means that a statistically robust data set can be gathered in a shorter period time for PMF

Source Apportionment

- More data allows for segmentation of receptor data prior to factorization
 - Data may be segmented based on seasons wind direction, wind speed and precipitation¹
- Hourly Data allows for confirmation of a factors source based on diurnal variability
 - Identification of traffic sources based on diurnal variability of sources and the effect of humidity on road dust²
 - Able to resolve braking factor and traffic emission sources²

1. Park, M., Lee, T., Lee, E., Kim, D.; Enhancing source identification of hourly PM2.5 data in Seoul based on a data segmentation scheme by positive matrix factorization. *Atmospheric Pollution Research- In Press*
2. Jeong, C., Wang, J., Hilker, N., Debosz, J., Sofowote, U., Su, Y., Noble, M., Healy, R., Munoz, T., Dabek-Zlotorzynska, E., Celoz, V., White, L., Audette, C., Herrod, D., Evans, G.; Temporal and spatial variability of traffic related PM2.5 sources: Comparison of exhaust and non-exhaust sources; *Atmospheric Environment.*; 198, (2019), 55-69

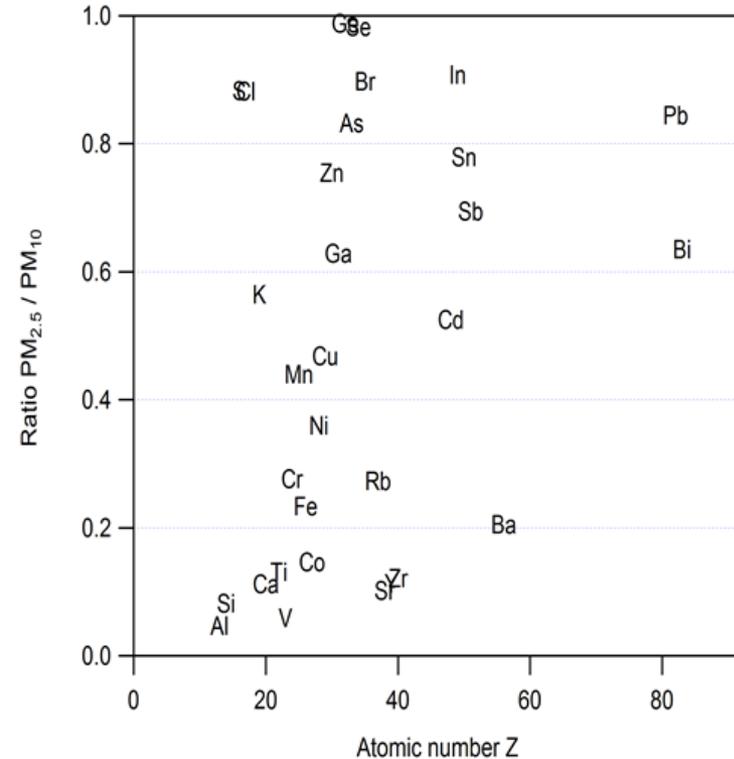
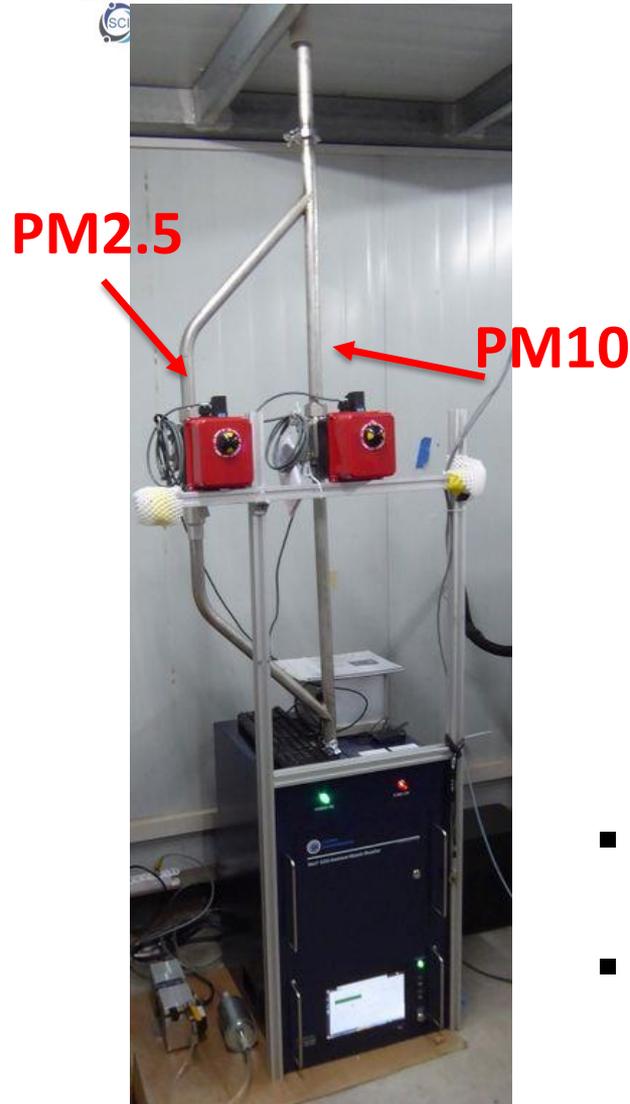
Source Apportionment

- Use of highly time resolved metals data allows for better resolution factors than could be identified based on longer time data³
- Highly time resolved data allows for easy correlation of factors with specific wind directions⁴

3. Wang, Q., Qiao, L., Zhou, M., Zhu, S., Griffith, S., Zhen Yu, J.; Source apportionment of PM_{2.5} using hourly measurements of elemental tracers and major constituents in an Urban Environment: Investigation of time resolution difference; *Journal of Geophysical Research: Atmospheres*, April 25th, 2018

4. Chang, Y., Huang, K., Xie, M., Deng, C., Zou, Z., Liu, S., Zhang, Y.; First long-term and near real-time measurement of trace elements in China's urban atmosphere: Temporal variability, source apportionment and precipitation effect. *Atmospheric Chemistry and Physics*, 18, 11793-11812, (2018)

Size Partitioning



- Sample Alternates between sampling PM10 and PM2.5
- Factors determined from both PM10 and PM2.5 data – different distribution of factors between size fractions

More Highly Resolved Metals Data

- 5 minute time intervals now available on the Xact
- Allows the instrument to be placed in a moving vehicle to identify metal pollution plumes

Conclusions

- Xact 625i can provide accurate metals analysis results in near real time
- Results are comparable to those obtained using standard laboratory techniques
- Results are useful in source apportionment and identification
- Instrument is used by researchers and environmental agencies throughout the world