

APPENDIX A

PAMS VALIDATION APPROACH USING VOCDAT

This procedure assumes that the data validation tool, VOCDat, will be used (remember to save the file often during validation).

1. After importing the data into VOCDat, check the species list for missing species by comparing the species list with the PAMS target list:

AIRS No.	Abbrev.	Compound	AIRS No.	Abbrev.	Compound
43203	ethyl	Ethylene	43232	nhept	n-Heptane
43206	acety	Acetylene	43261	mcyhx	Methylcyclohexane
43202	ethan	Ethane	43252	234tmp	2,3,4-Trimethylpentane
43205	prpyl	Propylene	45202	tolu	Toluene
43204	propa	Propane	43960	2mhpep	2-Methylheptane
43214	isbta	Isobutane	43253	3mhpep	3-Methylheptane
43280	1bute	1-Butene	43233	noct	n-Octane
43212	nbuta	n-Butane	45203	ebenz	Ethylbenzene
43216	t2bte	trans-2-Butene	45109	m/pxy	m/p-Xylene
43217	c2bte	cis-2-Butene	45220	styr	Styrene
43221	ispna	Isopentane	45204	oxyl	o-Xylene
43224	1pnte	1-Pentene	43235	nnon	n-Nonane
43220	npnta	n-Pentane	45210	ispbz	Isopropylbenzene
43243	ispre	Isoprene	45209	npbz	n-Propylbenzene
43226	t2pne	trans-2-Pentene	45212	metol	m-Ethyltoluene
43227	c2pne	cis-2-Pentene	45213	petol	p-Ethyltoluene
43244	22dmb	2,2-Dimethylbutane	45207	135tmb	1,3,5-Trimethylbenzene
43242	cypna	Cyclopentane	45211	oetol	o-Ethyltoluene
43284	23dmb	2,3-Dimethylbutane	45208	124tmb	1,2,4-Trimethylbenzene
43285	2mpna	2-Methylpentane	43238	ndec	n-Decane
43230	3mpna	3-Methylpentane	45225	123tmb	1,2,3-Trimethylbenzene
43231	nhexa	n-Hexane	45218	mdeben	m-Diethylbenzene
43262	mcpna	Methylcyclopentane	45219	pdeben	p-Diethylbenzene
43247	24dmp	2,4-Dimethylpentane	43954	nundc	n-Undecane
45201	benz	Benzene	43502	form	Formaldehyde
43248	cyhxa	Cyclohexane	43551	acet	Acetone (optional)
43263	2mhxa	2-Methylhexane	43503	aceta	Acetaldehyde
43291	23dmp	2,3-Dimethylpentane	43000	PAMHC	Sum of PAMS target compounds
43249	3mhxa	3-Methylhexane	43102	TNMOC	Total nonmethane organic compound
43250	224tmp	2,2,4-Trimethylpentane			

2. Run auto-screening checks found in VOCDat and print/save the results. Modify QC checks to best fit your data, if necessary.
3. Prepare summary statistics and print/save results. Inspect the statistics for common days with maximum or minimum values and note data ranges.
4. Inspect time series of all species (e.g., benzene, acetylene) and species groups (e.g., olefins, unidentified). Look for sudden dips or jumps in data, negative unidentified values, isolated high concentrations, pattern of decay (high concentration followed by slow tailing off), same concentration for several hours, and species that track each other and then suddenly change. Typically time series are prepared with the data in elution order so make sure to also plot a time series of species reported on different columns of the system (e.g., toluene and ethane) to look for column failures.
5. Inspect the following scatter plots and look for outliers¹:
 - Every species and species group versus TNMOC (and benzene - optional)
 - Benzene versus acetylene, toluene (typically correlate, with some toluene outliers where toluene is greater than benzene); cyclohexane (look for split in the scatter plot indicating misidentification)
 - Propane vs. propene (look for outliers), ethane (may correlate well)
 - i-butane vs. n-butane (should correlate)
 - i-pentane vs. n-pentane (should correlate)
 - 2-methylpentane vs. 3-methylpentane (should correlate with 3-methylpentane about 0.6 times 2-methylpentane)
 - Toluene versus 2,3,4-trimethylpentane, 2-methylheptane (look for misidentification)
 - Ethylbenzene vs. 1,2,4-trimethylbenzene (should correlate)
 - m-&p-xylene vs. o-xylene (o-xylene should be less than sum of m&p-xylenes), ethylbenzene (should correlate); styrene (should be less than the sum of xylenes)
 - Decane vs. undecane (look for high concentration outliers)
 - Formaldehyde vs. acetaldehyde
 - C- and t-butenes (should be 1:1; although this relationship is not observed at all sites)
 - Any other species that appear to have a set pattern
6. Inspect all fingerprints with a focus on odd data discovered during the above procedures (look for gaps in data, odd fingerprints, abrupt changes)
7. When flagging data as suspect or invalid, enter a comment describing why the action was taken.
8. Review comments in the log file that accompanies the VOCDat data file.

¹ These guidelines are pertinent to urban sites with a strong motor vehicle signature; rural sites or sites with strong industrial source influence may have different species relationships.