

COMPUTERIZED ENVIRONMENTAL ANALYSIS METHOD SELECTIONS

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The environmental analytical world has become a jungle of analytes and methods over the past fifteen years. From a relatively few simple methods for analyzing water quality parameters, elements, and organics prior to the mid 1970s a great proliferation of methods and lists of specific chemicals that cause environmental problems has mushroomed into existence. Now, there are hundreds of methods for hundreds of analytes. The problem is that many of these analytes are covered by multiple methods. This raises the question of which method should be selected for a given analyte?

The answer is not often a simple one. It depends on several important factors, each of which must be considered:

- * what analytical instrumentation is needed?
- * what environmental matrix is involved?
- * what interferences may be present in the samples?
- * what detection levels are needed?
- * how fast must the samples be processed?

One of the first considerations in selecting a method is the analytical instrumentation that is needed for the analysis. For example, in analyzing for 1,2-dichlorobenzene there are EPA methods that employ a gas chromatograph (GC) with a packed column and a photoionization detector (PID) (Methods 503.1, 602 and 8020). Three other methods use a GC with a packed column and a halogen specific electroconductivity detector (HECD) (Methods 502.1, 601 and 8010). Another (Method 502.2) has the variation of requiring a GC with a capillary column and a HECD. A third detector (an electron capture detector, ECD) is used with a GC and a packed column with Method 8120. The most selective detector is a mass spectrometer (MS) and there are three methods covered by the subject publication which use it (Methods 524.1, 524.2 and 624). The first and last of these (524.1 and 624) only require packed columns but Method 524.2 requires a capillary GC column.

Thus, if only packed column GC capability is available you may utilize Methods 502.1, 503.1, 601, 602, 8010, 8020 or 8120 (assuming appropriate detectors are available). If a laboratory has more sophisticated capillary column capabilities then Method 502.2 can be used (if an HECD is available). If a laboratory has GC/MS capabilities but the GCs have only packed columns then it can use Methods 524.1 and 624, but if it has capillary column capabilities with GC/MS then Method 524.2 can be

utilized. However, all of these methods except Method 8120 also require a purge and trap apparatus as the sample inlet to the GC.

Different matrices also require different methods. The methods have various modifications in sample preparation, instrumentation, and analytical parameters for different matrices. For example, EPA Methods 502.1, 502.2, 503.1, 524.1, and 524.2 are all suitable for analyzing the 1,2-dichlorobenzene example above in drinking water. But none of these are approved for analyzing 1,2-dichlorobenzene, or the other compounds they are verified for, in wastewater, ground water, soils, sludges, or wastes. EPA Methods 601, 602 and 624 are approved for wastewaters and EPA Methods 8010, 8020 and 8120 are approved for soils, sludges, ground water, surface water, wastes and other matrices.

Interferences are also important considerations in making method selections. For example, the analysis of halogenated compounds using electron capture detectors has the advantages of being highly sensitive and moderately inexpensive. But, ECDs are not very selective and, in sample matrices which have high levels of PNAs, phthalate esters and other oxygen, sulfur or halogen-containing compounds, the analyte's of interest may be masked by interfering compounds and result in false positive identifications. Thus, Method 8120 must be used with caution if interferences are probable.

Detection levels are another important factor. If the instrumentation at hand cannot reach desired detection levels by one method and different instrumentation using an alternate method will reach those levels then there is little choice but to use laboratories that have the instrumentation and expertise to reach the desired levels or else be satisfied with higher detection levels. Using elemental analyses as a different example, there are at least 4 U.S. EPA methods for analyzing for total chromium. Methods 200.7 and 6010 utilize inductively coupled plasma emission (ICP) spectrometry and have Method Detection Levels (MDL) of 7 ug/L. However, the instrumentation is expensive and not available at all laboratories. Direct aspiration flame atomic absorption (AA) spectrometry is more commonly available and EPA Method 7190 utilizes this technique with a MDL of 50 ug/L for total chromium. Method 7191 is a variation using a graphite furnace with AA and has a MDL of 1 ug/L for total chromium. Thus, if low detection levels are a major concern this latter method is the one of choice.

Sometimes samples may not be able to be processed quickly enough to avoid exceeding the maximum holding times (M.H.T.) of a method. In these cases if there is an alternate method that has longer M.H.T.s the integrity of the sample may be saved. The 1,2-dichlorobenzene can be used as an example again. All of the above methods used to analyze for 1,2-dichlorobenzene employ the purge and trap technique except Method 8120. The purge and trap technique has a M.H.T. of 14 days (except with unpreserved samples being analyzed by Methods 602 or 8020 -- then it is reduced to 7 days) but using Method 8120 the samples only have to be extracted within 7 to 14 days and the extracts analyzed within 40 days, thus providing a longer holding time if necessary. Unfortunately, not

many analytes are able to utilize techniques which allow this flexibility but, when it is available it can be useful in critical situations.

At Radian, we have developed an effective computer program that performs "free text" based searches simply and rapidly. ASCII text abstracts, summaries, sections of reports, or any other word processor-typed text can be strung together in files of any length and this program will perform "and/or" searches and present the summaries found. The format presentation is similar to hypertext searches. Pressing a highlight bar on a given title on the computer's monitor provides a window with the desired text in it which can be freely scrolled for browsing. And, the keywords entered for searching are highlighted in the text for easy referencing. Each "summary or section" that has been identified in the file can be browsed or written to a report file or printed.

This program has been combined with summaries from EPA's Sampling and Analysis Database. These summaries were compiled by William Mueller and David L. Smith at EPA's Risk Reduction Engineering Laboratory (RREL) in Cincinnati, Ohio. After extensive editing by Dr. Keith they were recompiled in files suitable for use with the above searching program, wrapped with menu-driven controls for easy use and prepared for general publication with a tutorial and a printed manual. In this format the data is now available as an inexpensive electronic publication from major commercial publishers in the USA and Europe. The title of this new publication is Sampling & Analysis Methods Database.

This is the first-of-its-kind "electronic reference book" on the U.S. EPA's Sampling and Analytical Methods. Appropriate methods can quickly be located using any number of keywords to focus on the specific needs of users. Each summary of an analyte and method is designed to be "self standing". In other words, each summary may be used by itself in a report or as a file in combination with other method/analyte summaries without loss of information. At Radian, we use this program to help our clients select the best methods for their specific needs. An example of a typical summary is shown in Figure 1.

In spite of the large number of method/analyte summaries in this publication (more than 650) not all of them are covered yet. There are still numerous methods for "specialized" analytes (for example, the chlorinated acids or the nitrogen-containing pesticides) and for the large number of semivolatiles compounds that have GC/MS methods. While many of these semivolatiles compounds are covered in the current status of this database they are not as completely covered as the purgeable compounds. If interest indicates that the work required to add these compounds would be warranted then they may be added in the future.

In the meantime, Sampling & Analysis Methods Database serves to help fill a need that many clients of analytical environmental services have. And, it demonstrates an important concept that any type of complex and voluminous information base can be readily edited and placed in a format where it can be made available to a mass market on a large volume/low cost basis similarly to current printed publications.

PRIMARY NAME: Aroclor 1242 (PCB-1242)

Method 8080

TITLE: Organochlorine Pesticides & PCBs MATRIX: groundwater, soils, sludges
water miscible liquid wastes,
CAS # : 53469-21-9 and non-water miscible wastes

APPLICATION: This method is used for the analysis of 19 pesticides and 7 Aroclor (PCB) mixtures. Samples are extracted, concentrated and analyzed using direct injection of both neat and diluted organic liquid into a gas chromatograph (GC).

INTERFERENCES: Solvents, reagents and glassware may introduce artifacts. Other interferences may come from coextracted compounds from samples. Phthalate esters are common interferences when using an electron capture detector (ECD) so all plastics must be strictly avoided. Exhaustive cleanup of reagents and glassware may be required to eliminate phthalate contamination. Use of a halogen specific microcoulometric or electrolytic conductivity detector will eliminate phthalate interference.

INSTRUMENTATION: GC capable of on-column injections and an ECD or a halogen specific detector (HSD). Column 1: 1.8 meter by 4 mm with 1.5% SP-2250 / 1.95% SP-2401 on Supelcoport. Column 2: 1.8 meter by 4 mm with 3% OV-1 on Supelcoport.

RANGE: 8.5 to 400 ug/L

MDL: 0.065 ug/L (in reagent water)

PRACTICAL QUANTITATION LIMIT FACTORS FOR MULTIPLYING TIMES FID MDL VALUE:

Matrix	Multiplication Factor
Groundwater	10
Low-level soil by sonication with GPC cleanup	670
High-level soil and sludge by sonication	10,000
Non-water miscible waste	100,000

PRECISION: $0.21X + 1.52$ ug/L (overall precision)

ACCURACY: $0.93C + 0.70$ ug/L (as recovery)

SAMPLING METHOD: Use 8 oz. widemouth glass bottles with Teflon lined caps for concentrated waste samples, soils, sediments and sludges. Use 1 or 2 1/2 gallon amber glass bottles with Teflon lined caps for liquid (water) samples.

STABILITY: Cool soil, sediment, sludge and liquid samples to 4 deg. C. If residual chlorine is present in liquid samples add 3 mL of 10% sodium thiosulfate per gallon of sample and cool to 4 deg. C. M.H.T. - 14 days for concentrated waste, soil, sediment or sludge. M.H.T. - 7 days for liquid samples. All extracts must be analyzed within 40 days.

QUALITY CONTROL: A quality control check sample concentrate containing each analyte of interest is required. The QC check sample concentrate may be prepared from pure standard materials or purchased as certified solutions. Use appropriate trip, matrix, control site, method, reagent and solvent blanks. Internal, surrogate and five concentration level calibration standards are used. The quality control check sample concentrate should contain aroclor 1242 at 50 ug/mL in acetone.

REFERENCE: Method 8080, SW-846, 3rd ed., Nov 1986.

Figure 1. A Summary of Aroclor 1242 Using Method 8080