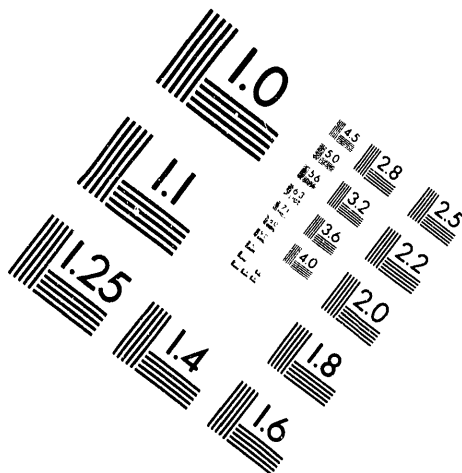
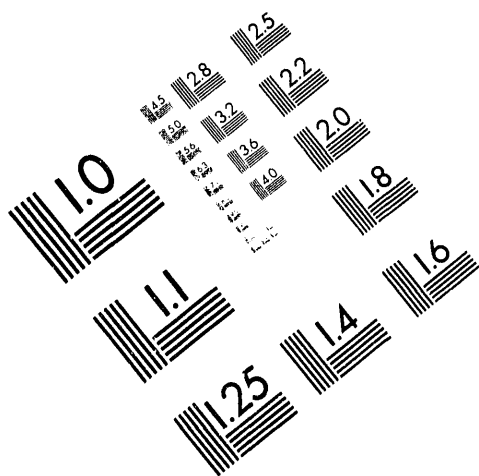




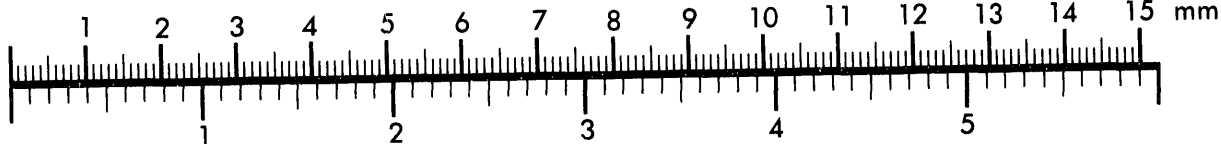
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Association for Information and Image Management

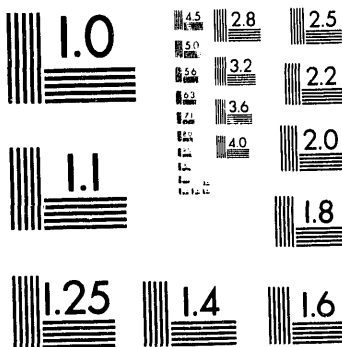
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Silver Spring, Maryland 20910
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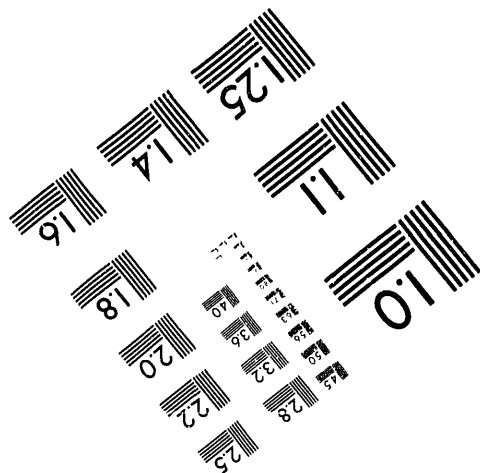
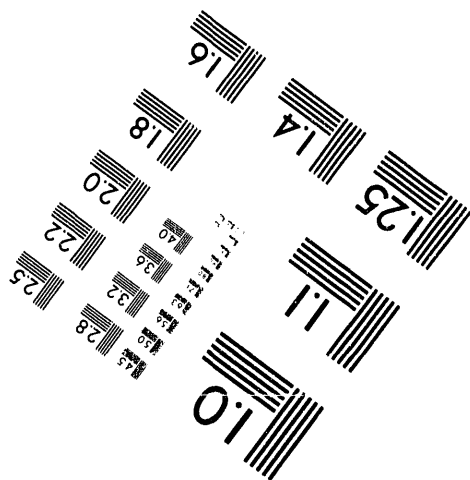
Centimeter



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AQUIS: A PC-Based Source Information Manager

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AQUIS: A PC-Based Source Information Manager

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ABSTRACT

The Air Quality Utility Information System (AQUIS) was developed to calculate emissions and track them along with related information about sources, stacks, controls, and permits. The system runs on IBM-compatible personal computers with dBASE IV and tracks more than 1,200 data items distributed among various source categories.

AQUIS is currently operating at 11 U.S. Air Force facilities, which have up to 1,000 sources, and two headquarters. The system provides a flexible reporting capability that permits users who are unfamiliar with database structure to design and prepare reports containing user-specified information. In addition to the criteria pollutants, AQUIS calculates compound-specific emissions and allows users to enter their own emission estimates.

INTRODUCTION

The Air Quality Utility Information System (AQUIS) is a database management system that operates on an IBM-compatible personal computer (PC) with dBASE IV. AQUIS is in operation at 11 U.S. Air Force facilities to assist with the management of source inventory, permit tracking, and estimating and tracking emissions. The system also provides environmental management personnel with information on regulatory requirements and other compliance information. Some of the facilities have more than 1,000 emission sources, which makes tracking and correlating emissions, sources, and permits a substantial task. AQUIS provides a single system for storing and accessing information previously available only in multiple, uncorrelated computer and hard-copy files.

AQUIS stores data for sources in about 30 different categories so that the data are tailored to the specific source of interest. This allows a large amount of detailed data to be stored about a source without making the number of individual data items to be considered for any source unduly large. Example source categories include internal and external combustors; solvent cleaning operations, including degreasers; four types of bulk storage tanks; fuel dispensing facilities; surface coating; wastewater treatment facilities; and abrasive cleaning. General Process and General Solvent Use categories are available for sources for which specific categories are unavailable.

DESCRIPTION OF THE SYSTEM

This section describes the development of AQUIS, its database structure, its features, and the procedures used to calculate emissions. It also describes the approach being taken to automate the estimation of emissions of air toxics.

System Development

AQUIS was initially developed to provide assistance to environmental managers at six installations. A data dictionary of elements needed to accomplish these tasks was compiled from the permit application forms and emissions reporting requirements applicable to these installations. Additional elements required to calculate emissions and define, locate, and identify the specific source of interest were included in the dictionary. Meetings were held with the user community to ensure that data needed for their internal management

procedures were included in AQUIS.

Source types in AQUIS include those described by permit application forms of the regulatory agencies as supplemented by categories identified during walk-through surveys of sources at these installations. Only stationary sources have been included.

The specific information and the level of detail requested on permit application forms vary substantially. The AQUIS data dictionary contains over 2,000 elements representing all of the permit information requested by each agency. It goes beyond the minimum data that would be required to calculate emissions and includes more than any base would need to fulfill its particular permitting and reporting requirements. A feature that would allow users to choose the fields displayed on data entry screens is nearing completion. This feature would retain a core of elements, including those required for emission calculations for all users.

Description of the Database

The following major categories comprise the first level of organization within AQUIS:

- Sources or events that generate air emissions,
- Control equipment,
- Permits,
- Emission points, and
- Connecting links between these items.

Sources/Events. AQUIS tracks a wide variety of data about emission sources. Although there are numerous definitions of "source," an AQUIS source is defined as a piece of equipment or a process that generates air emissions. The system does provide for the aggregation of identical sources under the same AQUIS identification number (AQUIS ID). Provision has been made for "events," which are unscheduled, aperiodic, or infrequent occurrences like spills. The same AQUIS ID can be used to identify any number of events so that all spills that occur during a year or month could be entered with the same ID. Data for sources are stored in a hierarchical set of files:

- Common data,
- Technology-specific data, and
- Fuels and materials data.

AQUIS tracks a basic set of data common to most sources: AQUIS ID, location, contact persons, and basic physical characteristics. The AQUIS ID is a unique number assigned to each source. Each source is physically tagged with the ID for unambiguous identification.

Beyond the common data, AQUIS tracks parameters that depend upon the type of technology being considered. Because these parameters vary considerably between source types, a technology-specific database is provided for each type.

Additional databases are provided to define fuels or materials and their consumption rates. These rates can be tracked for hourly, daily, seasonal, and yearly periods under maximum and average consumption conditions. The ability to store monthly consumption data on a rolling basis is being added. This feature will assist managers to report monthly VOC usage and emissions.

Control Equipment. Control equipment data storage is similar to that for sources. AQUIS stores a set of common data along with technology-specific data. Provision has been made for chemically speciated efficiencies to be associated with each control.

Permits. Permit information includes permit number, status, and about 10 data fields to track a permit's progress from submittal through reviews and revisions to approval and renewal. Based on discussions with users, 240-character text fields have been provided for notes on administrative matters. Related databases are available to record permit conditions, violations, permit fees, and fines.

Emission Points. AQUIS stores data on emission points, including the parameters needed for standard air quality models. Point, area, and volume sources can be defined.

Database Links. Sources, control equipment, emission points, and permits can be related in complex fashions. The AQUIS linking database stores the physical and logical connections among these entities in a fully flexible way so that none of the physical reality is lost. This linking capability is discussed below under **Linking**.

System Features

AQUIS is designed for use by environmental and air pollution managers, staff, and support personnel. A human-oriented interface enables users with minimal training to start using the system quickly. A hierarchical set of menus and windows allows users to access all of the functions within AQUIS. These functions include running standard or custom reports, viewing and updating data, adding data, and performing emission calculations. A standard set of keys to invoke AQUIS functions, such as Help or Define Range, on selection menus is available.

Before viewing data, the user can assign values to a set of parameters, such as Building Number or Source Category, in a selection menu. The values assigned determine which records are presented for viewing. When the user has selected more than one record (such as "all of the sources in Building 362"), an index of the selected records is displayed, along with several key data fields for each record. The user can then select to view any one of the displayed records.

AQUIS uses an active data dictionary that provides functional flexibility. For example, each time a data field is entered or altered, AQUIS checks the entered value against a valid range for that field. If the value entered lies outside the range, the program warns the user, who has the option of overriding the warning and entering the data into the system.

The active data dictionary also gives users control over the data fields presented in the selection menus. AQUIS provides an initial set of fields for each menu. If the user wants to select records by a different field, one keystroke accesses the data dictionary, which then lists all the data fields for that type of record. The user then selects the data fields of interest, and the system proceeds to select records on the user-defined basis. User's can choose to make their selections permanent. The capability to define the data to be displayed on a screen dynamically also depends on the active data dictionary.

AQUIS distinguishes blanks and zeroes in number fields. The system can thus distinguish missing data from true zeroes. This avoids potentially misleading information such as reporting zero emissions when the data are unavailable to make any emissions estimates.

AQUIS was developed with dBASE IV (version 1.1). Users are not required to know dBASE. The system is distributed via dBASE's Runtime version, which does not require the user to purchase a copy of dBASE or to have a license.

Emission Calculations

AQUIS can make emission estimates for many types of sources. The system estimates emissions only upon user request. In addition to the AQUIS-calculated emissions, users can store up to five additional emission estimates for each source-pollutant combination. For example, emission estimates calculated from emission factors required by a regulatory agency or developed by the user, a stack test, a material balance, and some "other" method could be kept and tracked along with the AQUIS-calculated emissions for a source. This capability is being enhanced by differentiating emissions estimates within a particular category by date, so that, for example, results from stack tests made in different years could be stored for future reference. In summing emissions, the user will be able to determine an order of precedence for defining which of the available estimates is to be used in the sum. When several estimates of the same type are available, AQUIS will choose the most recent.

AQUIS calculates emissions of the following pollutants: particulate matter (PM), particulate matter less than 10 μm in diameter (PM_{10}), sulfur oxides (SO_x), nitrous oxides (NO_x), carbon monoxide (CO), and volatile organic compounds (VOCs). For most source categories, the procedures used to calculate emissions are based on those given by the U.S. Environmental Protection Agency (EPA) in AP-42¹. If AP-42 presents alternative procedures, AQUIS uses the best alternative for which the needed data are available. For categories (currently five) not in AP-42, AQUIS implements procedures drawn from the literature or based on engineering judgment. For the General Process category, which is used for sources that have no specific algorithms, users can enter an emission factor and associated usage or process rates, and AQUIS will calculate the emissions.

If no factors are available in AP-42, AQUIS calculates PM_{10} emissions as a fraction of PM emissions. The fractions are taken from the EPA's VOC/PM Speciation Data System² or are based on the PM and PM_{10} emissions factors in AIRS³. Where appropriate, the fractions were chosen as averages of similar source types or

as the fraction for the most similar source.

For organics, AQUIS calculates the emissions of both the specific compound and the contribution of that compound to VOCs. Compounds on EPA's list of nonreactive organics are not included with the VOCs. For example, for a degreaser with 1,1,1-trichloroethane (TCA), AQUIS would calculate a zero VOC emission rate and a nonzero TCA emission rate because TCA is not photochemically reactive.

For each pollutant, AQUIS calculates both annual-average and hourly maximum emissions. For certain source categories, such as storage tanks, emission estimating procedures are intended to be used only for estimating annual emissions. In such cases, AQUIS lists the hourly maximum emissions as "N/App" to alert the user that the reason hourly rates are not calculated is because acceptable calculation procedures are not available and not because of a lack of data in the system.

Uncontrolled and controlled emissions rates are calculated for both time periods. Control efficiencies are generally taken from the individual control device files. Exceptions occur for some source categories, such as degreasers and abrasive blasters, for which integral controls are part of the source itself. In such cases, the AQUIS uncontrolled emissions include the effect of the integral controls, and the controlled emissions reflect the effect of additional add-on controls. The control device or devices used to control a particular source are determined from the Linking Table during the estimation of emissions.

AQUIS checks for three conditions during emission calculations and enters flags in the emission fields to inform users of these conditions.

1. If data are inconsistent or data needed to calculate emissions are not available, AQUIS alerts the user by entering "No Calcs" in the emissions fields. The use of "No Calcs" avoids the commonly used and incorrect default of zero emissions in such cases. Assistance in determining the reason for "No Calcs" is provided by distinguishing the data used in emission calculations by color on the data entry screens and by printing error messages to the screen and to a text file.
2. An "N/A" flag is entered when the user's data, although complete, cannot be found in an internal AQUIS database. This can happen, for example, when calculating emissions from tests of newer jet engines for which published emission factors are not yet available. In such cases, the user could make and enter their own estimates.
3. If data are sufficiently incorrect that a negative emission estimate results, AQUIS enters "Neg." in the emission fields.

In summing emissions, AQUIS treats all four flags (including the N/App flag) as zeros. A future revision will provide insight into the completeness of the emission sums by indicating the fraction of the sources summed that had flags rather than numerical estimates.

Linking

AQUIS offers full flexibility in linking any number of sources through any sequence of parallel or series control devices. It is necessary to link the data in a given control or source record with the corresponding data in other records in a manner consistent with the actual connections. For example, a source may simply be connected to a stack and be separately covered by a single permit; the appropriate source information needs to be linked to the corresponding stack and permit information. In the field, more complicated connections frequently occur among multiple sources, control devices, and stacks. Permits often cover more than one inventoried source. Flexibility in defining the possible linkages was needed to avoid complicated attempts to build all the likely connections among the four major information categories into the AQUIS system. The necessary flexibility has been created through a linking function that enables the user to define each link between the sources, control equipment, stacks, and permits.

The linking concept is illustrated in Figure 1. Links have been defined to connect source equipment to control devices, stacks, and permits. A control device, in turn, can be linked to other control devices, stacks, and permits. A critical feature of a link is its ability to accept multiple data records at both ends. This multiple linking capability allows the system to handle any number of sources connected through any system of interconnected control devices and stacks. Permits for single sources or for multiple sources and/or control equipment and/or stacks can be handled and tracked by the links.

Compound-Specific Emissions

When entering data, pure substances can be identified by their Chemical Abstract Services (CAS) numbers. This number provides a more precise identification of substances, particularly organic compounds, than long and often misspelled names. CAS numbers are used to identify nonreactive organic compounds. AQUIS uses its own set of CAS numbers, such as PM and NOX, to identify mixtures of interest in air pollution work that have no standard CAS numbers. In addition, certain mixtures widely used at Air Force facilities have also been assigned CAS numbers so that their contributions to total emissions can be readily tracked. Examples of these are "JP4" for JP-4 jet fuel and "PD680" for Stoddard solvent (designated PD-680 in Air Force applications).

Whenever CAS numbers have been entered for process materials, AQUIS calculates emissions of these materials in addition to emissions of the six criteria pollutants. For a TCA degreaser, for example, AQUIS would calculate a nonzero TCA emission rate and a zero VOC emission. The TCA rate would be identified as "CAS 71556," which is the CAS number for TCA, and would be summed with other emissions of CAS 71556 during report preparation.

AQUIS can carry any number of compound-specific emission rates for a particular source. For operations such as paint booths that can use a number of solvents, AQUIS calculates both the overall VOC emissions and an emission rate for each solvent. Summary reports can then be developed that give VOC emissions, as well as emissions of specific substances such as TCA or methylene chloride. If CAS numbers are missing, AQUIS tracks the associated emissions as emissions of "CAS" and assumes that the material is a VOC. Thus, the user can determine the fraction of VOC emissions due to compounds with unknown CAS numbers, some of which might be on EPA's list of nonreactive organics.

Users can also enter their own compound-specific emissions. Emissions of chromium from abrasive blasting of primers or of the various constituents of JP-4 could be entered into the database for individual sources and retrieved in summary formats.

The calculation of air toxic emissions is being automated. This effort is utilizing information supplied by McClellan AFB to support their air toxics inventory and to estimate fully speciated emissions for a large corrosion control (painting) facility at Robins AFB. Additional information is being developed from EPA's Air CHIEF⁴ and standard sources of EPA emission factors: AP-42 and selected "Locating and Estimating" reports.⁵⁻¹⁹

However, given the sensitivity of a process's toxic emissions to the precise materials used, the main source of data for making toxics estimates is coming from the Hazardous Material Information System (HMIS) database²⁰, which provides Material Safety Data Sheet (MSDS) information on a CD-ROM. The HMIS database is accessible through the National Stock Number (NSN), a 13-digit number used by the federal government to identify materials. Each material record in AQUIS has a provision for entering the NSN. The MSDS information in HMIS includes the composition of the material and can be used to decompose a compound into its constituent pure substances. However, the composition data in HMIS usually includes only toxic constituents, and thus the total percentage composition is less than 100%. In these cases, it is assumed that the constituents not listed are not air toxics. Additionally, percentage compositions summing to more than 100% have been found. In such cases, scaling to 100% is used to provide a reasonable estimate. When ranges are given, range midpoints normalized to 100% are used. Users will be able to add new data and change existing data.

The data in HMIS are being used to develop a database of material constituents. The constituents are the pure substances or toxic classes associated with a particular material. The data include the weight percents of the constituents which can then be used to speciate the emissions. In situations involving chemical reactions between materials, such as the application of polyurethane paints, some assumptions about the emissions of unreacted constituents are necessary. Additional databases, such as EPA's *Clean Air Act Air Toxics Data Base*²¹, have been used to develop another database of physical properties for the constituents needed to estimate emissions. These physical properties include parameters such as molecular weight, density, vapor pressure, and the coefficients for Antoine's equation.

Report Generation

AQUIS provides two reporting formats. A set of "standard" reports is available that print out all data fields. For standard reports, the user selects the data fields and associated values that will determine which records will be output. For example, the user could choose to report data on degreasers either with or without associated control device, permit, and consumption information. The user cannot, however, control the specific data to be output.

In "user-defined" reports, the user can determine which fields are output. For each type of record (for example, a technology-specific record for degreasers), the user can select which fields will go into the report, their order of printing across the page, whether the report is ordered by that field, and whether the field will be summed. These report formats can be saved for future use. A set of user-defined reports is supplied with AQUIS. The user can review, change, and delete reports from the set and create new reports to meet specific needs.

CURRENT SYSTEM OPERATIONAL STATUS

AQUIS has been installed at 11 Air Force installations. Each installed system includes a database of the sources and related permit information developed during site visits. As many as 1,000 sources have been inventoried for some facilities.

The emphasis by the users has been on identifying data gaps in inventory records to ensure that all sources — whether permitted or unpermitted, regulated or unregulated — are addressed and on ensuring that the information includes essential data on sources, operating conditions, control equipment, and stacks. Inclusion of chemical-specific (pollutant) information is essential for current and future uses of the system.

AQUIS has enabled users to respond to short-term inquiries about air pollution programs. One significant benefit of the system is its ability to generate comprehensive reports for a variety of requests in a short period of time. Inquiries about specific facilities or sources, source categories, and permits have been answered by using the standard or user-defined reports. Air pollution managers have been able to respond to regulator inquiries within a matter of hours, as opposed to several days, by having source counts, source information, and permit information available in a computer-accessible form. The system is also being used to develop annual emission inventory updates.

CONCLUSION

AQUIS is a functional but expanding system that has been installed with almost completed databases at 11 Air Force facilities. It contains little specific to the Air Force. It is very adaptable and should be applicable to other U.S. Department of Defense services or industries with a similar array of source types. AQUIS has proven useful as a management tool that can be used to help respond to the requirements of the new Clean Air Act and guide air pollution compliance programs.

ACKNOWLEDGMENTS

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REFERENCES

1. U.S. Environmental Protection Agency (EPA), *Compilation of Air Pollutant Emission Factors*, 5th ed., Supplement E, AP-42, Research Triangle Park, N.C., 1992.
2. EPA, *VOC/PM Speciation Data System User's Guide*, revised version 1.32, prepared by Radian Corp., Box 13000, Research Triangle Park, N.C., for EPA, Noncriteria Pollutants Programs Branch, Research Triangle Park, N.C., 1989 (available with IBM-compatible diskettes from Noncriteria Pollutants Program Branch).
3. EPA, *AIRS Facility Subsystem, Source Classification Codes and Emission Factor Listing for Criteria Air Pollutants*, Monitoring and Reports Branch and National Air Data Branch, Research Triangle Park, N.C., March 1990.
4. Ingram, A.L., and A.A. Pope, *Air-CHIEF CD-ROM*, Version 2.0 Beta, EPA, Office of Air Quality Planning and Standards (OAQPS), EPA, Research Triangle Park, N.C., April 1992 (available on a CD-ROM from OAQPS).
5. EPA, *Locating and Estimating Air (Toxic) Emissions of Carbon Tetrachloride*, EPA Report No. EPA-450/4-84-007b, 1984.
6. EPA, *Locating and Estimating Air (Toxic) Emissions of Chloroform*, EPA Report No. EPA-450/4-84-007c, 1984.
7. EPA, *Locating and Estimating Air (Toxic) Emissions of Ethylene Dichloride*, EPA Report No. EPA-450/4-84-007d, 1984.
8. EPA, *Locating and Estimating Air (Toxic) Emissions of Nickel*, EPA Report No. EPA-450/4-84-007f, 1984.
9. EPA, *Locating and Estimating Air (Toxic) Emissions of Chromium*, EPA Report No. EPA-450/4-84-007g, 1985.
10. EPA, *Locating and Estimating Air (Toxic) Emissions of Chromium (supplement)*, EPA Report No. EPA-450/4-89-002, 1989.
11. EPA, *Locating and Estimating Air (Toxic) Emissions of Manganese*, EPA Report No. EPA-450/4-84-007h, 1986.
12. EPA, *Locating and Estimating Air (Toxic) Emissions of Chlorobenzenes*, EPA Report No. EPA-450/4-84-007m, 1987.
13. EPA, *Locating and Estimating Air (Toxic) Emissions of Polychlorinated Biphenyls (PCBs)*, EPA Report No. EPA-450/4-84-007n, 1987.
14. EPA, *Locating and Estimating Air (Toxic) Emissions of Polycyclic Organic Matter (POM)*, EPA Report No. EPA-450/4-84-007p, 1988.
15. EPA, *Locating and Estimating Air (Toxic) Emissions of Benzene*, EPA Report No. EPA-450/4-84-007q, 1988.
16. EPA, *Locating and Estimating Air (Toxic) Emissions from Organic Liquid Storage Tanks*, EPA Report No. EPA-450/4-88-004, 1988.
17. EPA, *Locating and Estimating Air (Toxic) Emissions from Municipal Waste Combustors*, EPA Report No. EPA-450/2-89-001, 1989.
18. EPA, *Locating and Estimating Air (Toxic) Emissions of Perchloroethylene and Trichloroethylene*, EPA Report No. EPA-450/2-89-013, 1989.

19. EPA, *Locating and Estimating Air (Toxic) Emissions from Sewage Sludge Incinerators*, EPA Report No. EPA-450/2-90-009, 1990.
20. Defense General Supply Center, *Hazardous Material Information System (HMIS)*, Feb. 1992 (available on CD-ROM through Lexine W. Langley, NCTAMS LANT, Code N911.3, Norfolk, Va., 23511-5355).
21. Keith, L., and M. Walker, *EPA's Clean Air Act Air Toxics Data Base, Vol. II, Air Toxics Chemical and Physical Properties*, Lewis Publishers, Boca Raton, Fla., 1993 (available from CRC Press, Inc., 2000 Corporate Blvd., NW, Boca Raton, Fla., on IBM-compatible diskette).

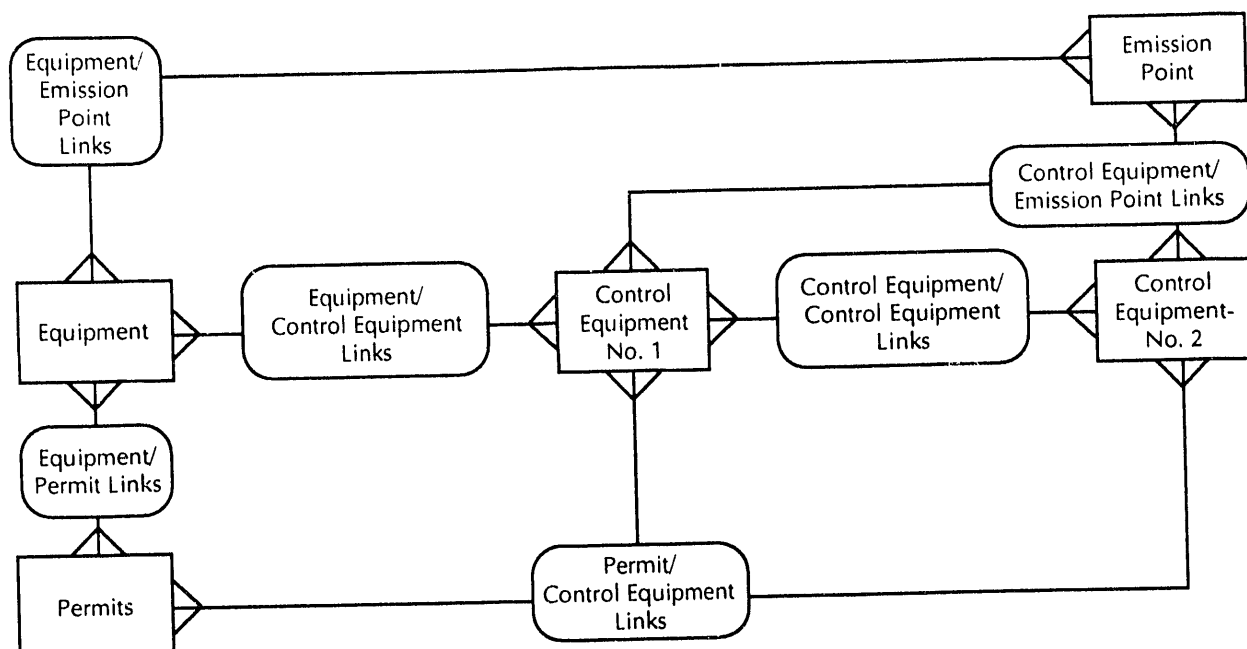


FIGURE 1 Structure of AQUIS links among data tables.

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