Contaminant Analysis Automation (CAA) Software

General Overview of the CAA Software

In their current implemtations, automated chemistry facilities are “islands of automation,” where automated systems are programmed to control specific devices that perform specific analysis operations. CAA software enables flexible, reconfigurable, and expandable laboratory automation.

The three main goals of software development for the CAA Program are to 1) define and test interface standards for implementing modular chemistry, 2) produce a representation of chemical analysis methods that is independent of any particular set of devices, and 3) develop an information model that captures and archives valid analysis data in an automated laboratory. To meet these goals, the CAA Program is developing software modules for the automated systems that perform laboratory control, user interface, and database functions.

Environmental Protection Agency (EPA) Method

CAA software is designed for processes that address all EPA criteria including the Contract Laboratory Program and Good Automated Laboratory Practice procedures.

Standard Analysis Method (SAM)

The CAA software allows the integration of SLMs into SAMs.

Advantages

The CAA system software provides standardized consistency and reliability in automated chemical analysis. It enables different analysis components to be used in a “plug-and-play” mode and eliminates the need to reprogram the task sequence controller (TSC) as different components are added or removed.

General Description of the Software

CAA system software is written to coordinate the interaction of the TSC, the human/computer interface (HCI), the laboratory information management system (LIMS), and the system database with other standard laboratory modules (SLMs). The TSC provides supervisory control of the automated modules on the laboratory bench, the HCI provides an intuitive interface with the system operator, the LIMS performs an interface between the SAM system and the analytical laboratory database, and the system database performs information storage and retrieval including chain-of-custody information and data archiving.

SLMs are “plug-and-play” building blocks for the automated laboratory. Each SLM can perform a subset of the operations required to implement complete chemical analysis methods. SLMs must conform to a set of standards. These standards include capabilities for external communications, remote control, and automated material transports. These standards can be captured as a set of interactions between the automated laboratory control system and the SLM.

An example of such an interaction is the transport of material into an SLM. The CAA Program has developed a draft SLM interface specification that defines the interactions between an SLM and the TSC. In addition to the SLM interface, we have defined a format for describing the capabilities of an SLM to the TSC. The common interface and the data set of the unique characteristics provide a completely data-driven interface to the SLM. This allows SLMs to be dynamically added and removed from the system without reprogramming the TSC.

The system database contains information about the system, the information needed for the processing of samples, and the information generated by the processing

and analysis of samples. The database is object-oriented, allowing the flexibility needed to model the system and its operation. A LIMS is interfaced with the CAA system through the database. Ultimately, with complete implementation, the LIMS would be used to generate reports as well as to log samples into the system, track samples, and respond to general queries about the system.

The operator enters samples into the system through the HCI. Each analysis method is programmed as a hierarchical script of operations and is downloaded to the TSC as an executable process script. The TSC executes these hierarchical scripts by expanding them into the set of elemental operations to be performed by SLMs in the laboratory. The TSC will then select an SLM to perform each operation based on the availability of the SLMs (as described in the characteristics data set), sample processing priorities, and any device selection criteria specified in the script. Selection of the SLM to perform an operation is made at run time; thus, redundant SLMs may be added to the system at any time to increase sample throughput. It is the responsibility of the TSC to ensure that all material transports are performed for the selected SLM and to initiate the operation of that SLM.

In addition to executing the necessary operations, the processing of the script includes archiving the necessary data into the database and notifying the HCI of relevant status and state changes. When the operation is complete, the TSC will determine the next operation to execute and again select the appropriate SLM and material transports. This continues until the entire analysis script is completed. The TSC may execute any number of analyses in parallel and therefore must ensure that system resources and devices are managed appropriately to avoid conflicts or holdups as the script is processed.

Status

The TSC is in the prototypical stage with some development still remaining.

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