Mixed Environment Support in OpenLab CDS

Introduction

This white paper clarifies the application and boundaries of the "mixed environment" concept in OpenLab CDS.

OpenLab CDS currently targets routine analysis workflows in the pharma and chemical and energy quality control market segments. Many laboratories perform different types of analyses. As a result, labs would like to use OpenLab CDS for some applications while continuing to run other analyses where the workflows are not supported by OpenLab CDS. They may do this with individual workstations or prefer to use a distributed, networked configuration.

This networked configuration is called a mixed environment architecture, which supports OpenLab CDS, OpenLab ChemStation, or OpenLab EZChrom, networked workstations, analytical instrument controllers (AICs) and clients with a shared OpenLab data management system that includes shared services and storage as shown in Figure 1.
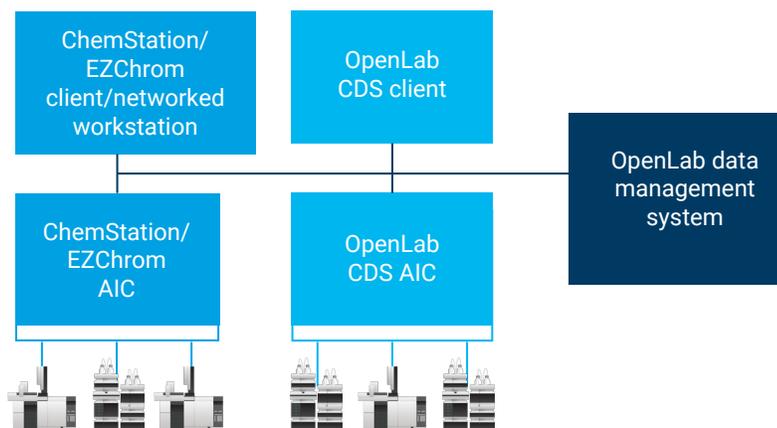

Figure 1. OpenLab mixed environment example

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What is the advantage of a mixed environment?

A mixed environment supports a heterogeneous CDS network deployment. Customers can take advantage of the advanced-usability features of OpenLab CDS, including new compliance features, while running workflows or instruments that are not supported in OpenLab CDS. They can also experience the additional benefits of a networked system with its central administration and repository. The advantages are outlined here in a series of examples:

– Example 1: A laboratory wants to use OpenLab CDS but must also perform advanced method development and/or purification workflows. OpenLab CDS does not support advanced method development, including UV library searching, or all fraction-collection workflows, including mass-based purification. A mixed environment deployment supports a networked OpenLab CDS system with its associated OpenLab backend along with attached ChemStation AICs or networked workstations.

– Example 2: A laboratory wants to use OpenLab CDS but has non-Agilent instruments that are not currently supported in OpenLab CDS. However, these instruments are supported in OpenLab EZChrom. The laboratory can deploy a networked OpenLab CDS system and attach an EZChrom AIC or networked workstation with the required third-party instrument control.

Note that data generated[1] in EZChrom can be opened in OpenLab CDS data analysis.

– Example 3: A laboratory has a small number of instruments that are used for "process control," i.e., they continuously monitor a sample stream and/or automatically adjust the sampling based on previous results. The laboratory can deploy a networked OpenLab CDS system for the instruments doing lab analytical work and attach an EZChrom AIC or networked workstation for the process control systems.

When is a mixed environment appropriate?

A mixed environment can be applicable if a laboratory is interested in rolling out OpenLab CDS, but also needs:

– Support of an instrument or module that is not yet supported with OpenLab CDS (see OpenLab CDS instrument support FAQ page for details)

– Application add-ons that are not supported in OpenLab CDS (see Chromatography add-ons page for supported add-ons)

– Part of a phased migration plan, including the ability to access complete historical information from data generated in either EZChrom or ChemStation

– Access to complete historical data due to data retention policy

– Customized solutions developed using either ChemStation macros or the EZChrom automation tool kit

Compatibility

The compatibility refers to the ability to run a ChemStation/EZChrom AIC and client with the OpenLab data management solution that is also used with OpenLab CDS.

Please see OpenLab ChemStation, OpenLab EZChrom, and OpenLab CDS requirements for details on what versions of OpenLab CDS and either ChemStation or EZChrom are supported with a specific OpenLab data management system deployment.

Note that it is not possible to have both EZChrom and ChemStation in the same mixed environment.

Also note that for EZChrom users needing to open data in OpenLab CDS, we require the use of the OpenLab EZChrom migration tool, which is available in your Agilent SubscribeNet account.

[1] See "Import EZChrom data" in OpenLab CDS Help & Learning for details.

Deployment of a mixed environment

When you deploy a mixed environment, you must take the following aspects into account.

Installation and configuration
– You must not deploy OpenLab CDS clients and ChemStation/EZChrom clients on the same computer.

– When you decide to deploy a mixed environment, install the OpenLab data management system first, including shared services (required for OpenLab ECM deployments). Then install the ChemStation or EZChrom AICs and clients as needed.

– Users, roles, and system settings can be administered centrally from any control panel.

– Configuration of instruments and projects must be done on a client or AIC where the corresponding application is installed, for example:
  • Use the control panel of an OpenLab CDS client to manage instruments and projects that are controlled and used by OpenLab CDS.
  • Use a control panel on a ChemStation client to configure instruments that are controlled by ChemStation.
  • Use the control panel of an EZChrom client to manage instruments and projects that are controlled and used by EZChrom.

– It is recommended to use a structure in the Instruments section of the control panel that helps you differentiate the instruments based on the application by which they are controlled (Figure 2).
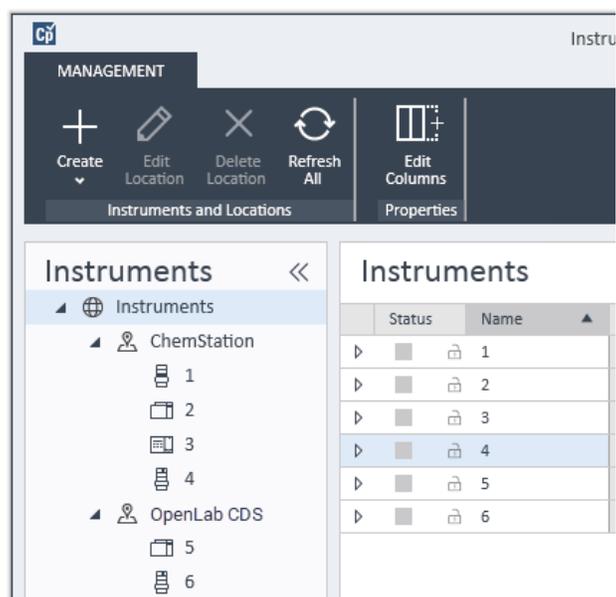

Figure 2. Instruments section in OpenLab control panel.

– We recommend creating application-specific roles and assigning them to the respective user of the applications. If users need to work with multiple applications, you should assign to them the specific roles for each application. Example: If user A needs to work with OpenLab CDS and EZChrom, assign an OpenLab CDS user role and an EZChrom user role.

– During routine work, use the ChemStation clients to access instruments that are controlled by a ChemStation AIC, and use OpenLab CDS clients to access instruments controlled by an OpenLab CDS AIC.

– Always launch and close instruments from the same application. For example, do not launch an instrument from a ChemStation client and close it from an OpenLab CDS client, or vice versa.

Data sharing
All applications in the mixed environment share the same storage that is provided by the OpenLab data management system. This allows you to open data generated in either ChemStation or EZChrom with OpenLab CDS.

Data from ChemStation revision C.01.01 or later can be loaded directly in OpenLab CDS.

To open ChemStation data in OpenLab CDS, you must:
– Configure OpenLab CDS to provide a project pointing to root folder where ChemStation data is stored (1), or move existing ChemStation SSZZip archives from their current location to an OpenLab CDS project results folder (2).

– Start the data analysis client in OpenLab CDS, either in the new ChemStation data (1), or an existing OpenLab CDS project (2).

– Open the ChemStation data (read only).

– Upon processing ChemStation data with OpenLab CDS, a new result set will be created next to the ChemStation SSZZip archive.

If OpenLab CDS is connected to OpenLab ECM, you can simply load the existing ChemStation SSZZip archives from their current location (see special aspects of working with OpenLab ECM 3.x).

EZChrom data and methods contains some attributes that are unique.[2] To successfully open and use this data in OpenLab CDS, it must be migrated to align with the OpenLab CDS capabilities.

A migration tool is available to support the migration of data and methods to a format that can be used by OpenLab CDS.

To open EZChrom data in OpenLab CDS, you must:

- Use the OpenLab EZChrom migration tool to migrate data from OpenLab EZChrom projects to OpenLab CDS.

- Start the Data Analysis client in OpenLab CDS; either in the newly migrated project (1) OR an existing OpenLab CDS project (2).

- Open the migrated EZChrom data (1) or browse to the migrated EZChrom project and open the migrated project data (read only).

It is not possible to open OpenLab CDS results in ChemStation or EZChrom.

Conclusion

By adopting the mixed environment approach, laboratories can leverage OpenLab CDS where applicable to continue to perform other analyses for which the workflows are not supported by OpenLab CDS. This provides lab managers with the flexibility to plan a system migration while minimizing disruptions to ongoing work.

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[2] For example, signal names and user-defined scaling of data.