Data Management Requirements for the Lab of the Future

The WTW-IDS-Gate – an open System for GxP-compliant Data Handling

This white paper describes the future-oriented data management of electro-chemical measurement parameters for the direct connection to database systems using an open REST API

Every modern lab poses the question whether working with a lab logbook is still keeping up with the times. In the course of digitalization of data, the handling of documents as hard copies is more and more frequently questioned and in times of COVID 19 and "the Home Office", the decentralized evaluation of measurement data is becoming even more important.

While the "Internet of Things" in the form of various Smart Home applications has already begun to enter our private surroundings, for many labs, digitalization is still at the beginning.

How can I ...

... replace the lab logbook?
Laboratory Manager

... achieve GLP conformity?
QM manager

... create data security
IT specialist

Data Management Requirements for the Lab of the Future

1. The requirements for the measurement values in the lab

... from the viewpoint of the Laboratory Manager:
The requirements in the lab have changed regarding the measurement data in so far as not only the measured value for the scientist/lab technician bears importance, but also the Quality Management and the IT department has expectations of the measurement data.

The complexity of the requirements can be demonstrated using this simple example. It is important for a "product" that the pH value is neutral, meaning at 7. In quality control, the pH value is determined and documented. To do this, the value is read from the display of the meter and manually entered into a lab logbook. In order to be able to later prove that the product was really pH neutral, the time of the measurement as well as the name of the person who took the measurement are entered as well. Finally, the person responsible for the measurement signs off and authenticates the accuracy of the data.

... from the viewpoint of the QM Manager:
In order to provide proof for the "accuracy" of a measurement value, it is necessary to also add the measurement conditions, e.g. the temperature, the meter, the calibration and sensor data.

For a subsequent digital processing of the data, all changes must be tracked using an "audit trail" and transparently documented, i.e., the measurement data must not be modifiable and it must be ensured that all information (meta data) associated with the measurement value are assigned correctly. Only this will make the dataset GLP-compliant and the quality management requirements are met.

... from the viewpoint of the IT Specialist:
Requirements regarding data formats, transmission systems and data security are essential for electronic data processing and the evaluation and storage of the datasets. For every manual process or transmission of data, input errors and manipulation can falsify the measurement value or corrupt the data. For sensitive data, special encryption technologies and security measures are required to protect the anonymity. All this must be taken into consideration and documented with a simple pH measurement that lasts three minutes.
In modern labs, a process must first be defined that will be reflected in the LIMS. The LIMS will then place an order as to WHO, WHEN, WHAT, HOW something is done.

2. Capturing measurement values using WTW IDS sensors

Measuring system requirements
A classic measuring system consists of a pH measuring meter and a compatible analog measuring sensor, which sends an analog high-ohm mV signal to the measuring meter. In the measuring meter, the signal is converted to a digital signal, displayed and/or stored. Modern meters communicate using a "smart" sensor, which already contains analog measurement values that have already been digitalized in the sensor; therefore, measurement values can be

A classic pH measuring system

transmitted to the measuring meter in digital format. The digital measuring system is a lot less sensitive to interference during data transmission caused by environmental influences (e.g. electric smog or cable length). Xylem Analytics has designed the IDS sensors so that there will not only be a signal conversion inside the sensor, but that calibration data, calibration logs and serial numbers are stored in the sensor head for the unique identification of a sensor. This eliminates the need for a parameter-specific meter, as the sensor transmits all important data for that parameter when connected to the meter. The measuring meter is therefore a multi-parameter meter, which can manage up to three sensors, depending on the number of input channels. The function of the meter is limited to the calibration routines, the memory management and the measurement value display of the different IDS sensors.
In another development step, the IDS sensors were equipped with a plug head and installable radio modules, which made sensor cables redundant. Thus, the samples to be measured no longer have to be taken to the measuring meter but instead, the measurement with the sensor takes place remotely, so long as the measuring meter is located in the radio range. A clear advantage that simplifies the measurement process and also allows for a safe measurement due to the sample analysis being made in situ.

With IDS sensors, the analog measurement values are already digitalized in the sensor (top left).

Cable-free transmission of measurement values via radio modules – for example in the exhaust.

## 3. The IDS Gate – from sensor into the LIMS

The IDS Gate allows a new, future-oriented method for capturing measuring values. The general principle of the system is shown in the figure on the subsequent page.
As digital data management is subject to regulations, such as GxP or FDA 21 CFR Part 11, manufacturers have been trying to meet these regulations in different ways in their current measuring meters. This way, they stick with "island solutions" and pursue their company-specific philosophy during the implementation. This starts with simple meters without storage all the way to server-supported total solutions in their own product portfolio.
The IDS Gate pursues another, free approach using an open REST API interface. As described above, the

IDS radio electrodes have a unique serial number. After the calibration process, the calibration data will also be available in the sensor. With the software in the IDS Gate, it is able to receive measurement data and meta data, such as user name, sample name, calibration data and serial number. The data transfer is done wirelessly. The meta data are connected with the measured value, the temperature and a time stamp. This data-package is ready to be taken from the LIMS . This fulfills the first part of the GxP requirements, the capturing of the data. The second part, the recording, archiving and the reporting of the test results is taken over by the LIMS of the user in larger companies. For smaller companies, who work without LIMS, the data can also be

IDS sensors and barcode reader supply data and meta data

Gateway/API-Interface
- merges data and meta data
- sets timestamp
- data exchange in JSON format

LIMS recalls data https:// Output as PDF/A

Visualization in Browser

transferred into Excel. More about this subject in part 4 of this article. At the start of the work, the measuring sensor is calibrated on any IDS measuring meter. After that, it is available for the measurement task. Sample data as well as user data can be transmitted in advance in the API or individually during the measurement process via a bar code reader. Confirming a measurement value on the radio module transmits the measurement data and meta data to the API of the IDS Gate and will receive a time stamp. This makes the data available for an external database. This external database can be a LIMS or e.g. an Excel database. Now, the LIMS retrieves the data important for its process sorted by its priority; for example, all data belonging to a certain user, which were collected at a certain time, or those that belong to a sample number etc. For the user to know which measurement value he selects during the measurement process, there is a browser-based "Status Viewer" that displays the most important data in real time on any output meter, such as a laptop, smart phone, tablet etc
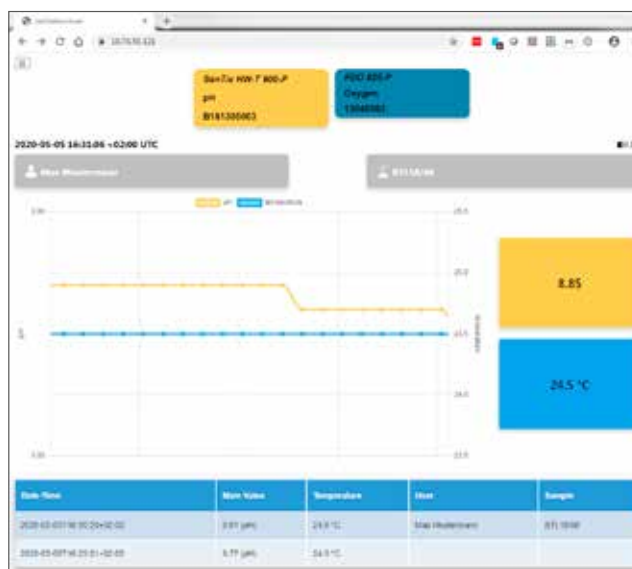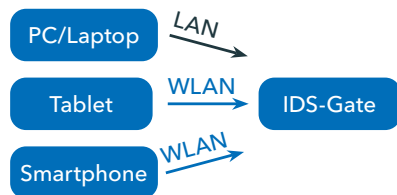

Functional principle of the IDS Gate solution (above)

Status Viewer in the browser (below).

Example for an Excel import (right, Page 5).

# 4) For the IT Specialist: This is how the IDS Gate works

There are two ways to connect the IDS Gate to a network:

1.) Direct connection via LAN and WIFI: The IDS Gate assigns an IP address to the connected meter.

2.) Connection to the local network: The IDS Gate is connected at the LAN interface ETH1 via a LAN cable to the local network. The DHCP server of the local network assigns an address for the IDS Gate as well as for a meter connected via LAN or Wireless LAN (desktop, laptop, smart phone or tablet).
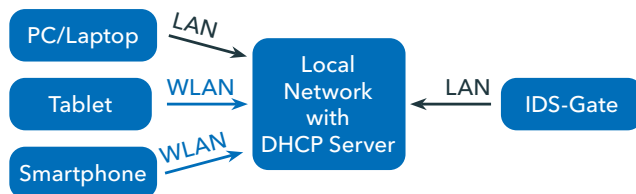
The IDS Gate API

The IDS Gate can be completely remote controlled via a REST API. A documentation of this API can be retrieved directly by the meter. The implementation takes place by simply entering *https://<ip-adresse>/api-doc/v1* into any browser (see figure on top right). The browser will then display an interactive documentation (Swagger UI) with the description of the API. In this documentation, the IT Specialist will find all data and actions needed to include the IDS Gate in a LIMS. Furthermore, with this Swagger UI, you can also directly test any API endpoint provided by the IDS Gate. For the beginner, the functionality of this API can be explained in a way that information and conditions (e.g. measurement values, current user of a sensor, time, etc.) can be read via **GET**. Actions (e.g.

connecting a sensor, assigning a sample ID, updating software, setting the time server, etc.) can be executed via **POST**.

Data import into Excel

For those not using a LIMS, but who wish to store their data for subsequent evaluation, there is the possibility to retrieve the data from Excel and to store it as they wish in Excel format. What is important here is that the data are not imported as a fixed string such as a CSV file but instead, all available data is retrievable in a format legible for a human (JSON), which the user can then filter as per his wishes. The Excel tool Query helps merge data from several data sources into one single target database or table. This is directly available in Excel 2013 (add-on must be installed) and all later versions of Excel.

Example for an Excel import.

Data security:
All data is transmitted via https. This ensures two things: First, the data cannot be read during the transport between IDS Gate and client (e.g. LIMS or Excel). Second, and this is much more impor-tant, https ensures, that the data retrieved by the client (e.g. LIMS or Excel), actually originate from the IDS-Gate. This ensures that nobody can introduce manipulated measurement values into the LIMS.

5. An example from the field

Mr. Maximilian Küppers, Chemical Lab Technician with Bayer AG Research & Development, Crop Science, concluded the following after having integrated WTW IDS radio sensors with the new IDS Gate into the company's proprietary LIMS system:
"An important advantage of the IDS system is the ability to work without cables. This creates a clean and safe work environment. If you use the sensors in combination with the IDS Gate, this creates another advantage due to the electronic measurement value collection. The "IDS Status Viewer" provided a preview of the measurement values on any meter in the network. Here, you can also see the sequence of the respective measurement value, which is a great help, for example when setting a pH value. With this system, you can process the measurement values further as you wish: There is the possibility, to store the data by creating a PDF as a CoA (Certificate of Analysis) on paper.
This option also allows working in an environment with hybrid raw data definition. In addition, you can of course work completely digitally and store the measu-rement values – as shown in the example – directly and without complications in a LIMS or in a table calcula-tion software. Here, there is the extra advantage that the measurement data is directly connected to the calibration log. Calibration and maintenance intervals can also be managed using the LIMS. Using this function also allows the setting, that only sensors with a valid calibration can be used for the generation of the measurement value.
The IDS Gate is an excellent option to start digitalizing a lab, as it can be introduced very simply and step by step."

Read the entire interview:

https://www.xylemanalytics.com/ File%20Library/Resource%20 Library/WTW/04%20Flyers%20 Brochures/ENG/Flyer_4_Interview- IDS-GATe_182-KB_En-pdf.pdf

Learn more about our IDS Gate.

https://www.youtube.com/watch?v=KgwyhFPjeXg

/wtwde
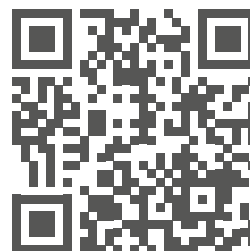
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