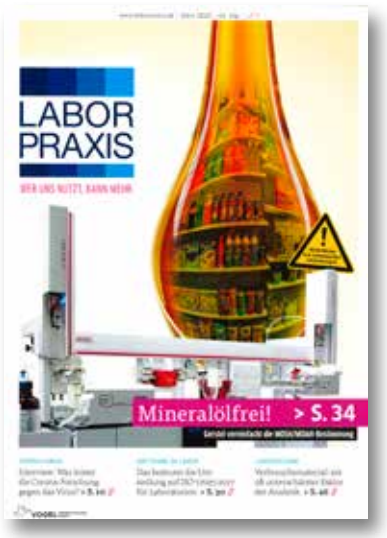
Data in the lab of the future

Assignable, real time, readable, original and correct

The WTW IDS Gate – an open system for GLP-compatible data handling in the lab

A joint Xylem Analytics Germany GmbH and Bayer AG project

Interview with Maximilian Küppers, Lab Chemist with Bayer AG Research & Development, Crop Science. First published in German language in Laborpraxis, March 2020



Maximilian Küppers is a skilled Lab Chemist and has been working on performing registry-relevant GLP studies to characterize the environmental characteristics of pesticides since 2016.
Since 2018, he has been part of a project team with the goal of modernizing the IT system landscape of the labs in environmental safety functions at Bayer AG Division Crop Science.
In addition, Maximilian Küppers is studying Chemistry at Zuyd University of Applied Science in Heerlen, NL.

Data in the lab of the future: assignable, real time, readable, original and correct

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Question: Mr. Küppers, can you tell us something about yourself as well as your job?
Answer: I work for Bayer in the area of chemical pesticides. In the course of environmental studies, my colleagues and I make sure that pesticides and their degradation products are not harmful for humans, animals and the environment. During this work, I deal with a great variety of environmental media. Among others, I regularly work with soil under aerobic and anaerobic conditions, water/sediment systems as well as buffered nutrient solutions for plant propagation in hydroponic cultivation.

Measuring the pH value using WTW IDS wireless sensors in a potato plant

Which mesured parameters are relevant for you?
In the context of the environmental media I just listed, the pH value, the oxygen content and the redox potential are of special interest to me. A common question, which can be answered by these physical measurements, for example, would be: "Is the ventilation of our hydroponic testing systems set strong enough and does the nutrient solution offer the ideal pH value for these plants?" or, when simulating the conditions of flooded fields, e.g. in rice cultivation: "Is the soil that is covered by water already anaerobic?"

Xylem Analytics has been offering high-quality meters for electro-chemical parameters for decades. In addition to the cabled IDS sensors, you also use the digital IDS sensors with radio transmission. Is there a reason for this?
When I first saw the IDS sensors, I was immediately convinced. Although, the "internet of things" has already moved into our private homes as various SmartHome applications, such as robotic vacuum cleaners and light and heating controls, we are still at the beginning of digitalization in the lab.
In my daily work, we are often faced with the necessity to perform several physical measurements in one testing system. This result in us having to sort all connecting cables at the beginning of our work day – a time-consuming and very unpopular work step. The new wireless radio sensors allow a significantly more comfortable process for this step. Furthermore, the system is very compact compared to the others. Also, with outdoor measurements, my colleagues and I have had good experiences with them. The pH measurement of the sediment of a lake can be taken by one colleague directly in the water, while another colleague remains on the shore and notes these measured values.

Xylem Analytics offers the "IDS Gate" for LIMS-compliant data transmission, a gateway with an open interface (REST API). This is used to transmit the measured data directly from the sensor into a data capturing system, without a detour via an instrument. Which requirements does the entire

measuring system need to meet regarding data security?

In order to ensure data security, the captured measured data should be assignable, readable, original and correct (ALCOA principle). Assignable means that the measured date contains information regarding the point in time the data were taken as well as the details of the person who conducted the measurement. Correct means that the measuring data can neither be altered nor deleted after the capture. With the IDS system, the user cannot delete measuring values once they are captured. The data set is then only available for a certain time period (7 days with us) to be picked up by our LIMS.

Due to the fact that the captured measured values are transferred directly into the LIMS, there is no way of manipulation during the import/export of CSV files on a workplace computer. Therefore, manipulation of the values, before they reach the LIMS, is no longer possible.

And how are the other ALCOA criteria fulfilled: real time, original and readable?

A timely documentation of the data is natural for this system, as a valid measuring date can be printed just a few seconds after the measurement is conducted. This measurement date is accepted as original by a handwritten or electronic signature. As the data is saved in the manufacturer-independent JSON (JavaScript Object Notation) format, their Readability can be ensured for decades to come.

Especially when data are further processed in a third party system like LIMS or EXCEL the further steps (in LIMS or EXCEL) need to be documented and validated. The system is a great basis for this, as there is the possibility to record a freely selectable sample identification number via a bar code scanner, as these numbers can also be used as a reference in the system used for further processing.

Question: The measuring system consists of radio sensors and the IDS Gate. How can you ensure GLP conformity?

A complete measurement data set in JSON format, consisting of time stamp, measured value, user as well as the serial number of the sensor used and a link to its current calibration date are available at the API of IDS Gate. This measurement data set can be transferred into lab information systems (LIMS) and processed there with very little effort. With this procedure, the main benefit is the audit trail of the LIMS, which clearly documents all further processing with a time stamp and user. Furthermore, there is the possibility to retrieve the measured values from the IDS Gate via a standard function of the common table calculation programs.

In addition to the listed JSON file, a PDF-A file is created on the IDS Gate, which contains the same measurement data set. This also provides for a direct printout of the PDF document as an analysis certificate (CoA). The multitude of possibilities of the measured value output allow the use of the system in environments with a variety of documentation requirements all the way to the GxP environment.

GxP conformity is given if the requirements of data security are met.

Why is the data format important?

In addition to working at the lab, I am also involved in an IT project at Bayer. The goal of this project is to save measuring results from the lab in structured form to facilitate the path for received evaluations via DataScience. The basis for this is that the values deliv-

ered by the measuring devices are sent in a file format which allows the readability of these values across a long time period and, if possible, without the need for additional software. The system developed by Xylem Analytics delivers the measured values in the JSON format, which offers several advantages. First, it has a simple data structure and format definition, so that it can be read by anybody, even people without IT experience. Furthermore, this format represents a great prelevel of the Allotrope format, the industry standard for the capture, exchange and administration of lab data.

How would you summarize the advantages of the system for your purpose?

An important advantage of the IDS system is the possibility to work wireless. This results in an organized and safe work station. If you use the IDS wireless sensors along with the IDS Gate, this is another benefit due to the electronic capture of measured values. The IDS status viewer provides a preview of the measured values in any device in the network. Here, you can also see the history of the respective measured value, which is especially helpful, e.g. when adjusting a pH value. You can further process the measured results any way you need to with this system: There is the option to save the data in hard copy by creating a PDF as a CoA (Certificate of Analysis). This option also allows working in an environment with hybrid raw data definition. Also, you can work completely digitally and save the measured values directly and without complications in a LIMS or in a table calculation software, as shown in the example. Here, there is the additional advantage that the measured data is directly connected to the calibration protocol. Also, you can maintain calibration and maintenance intervals by means of LIMS. The use of this function also enables the setting that only sensors, which have a valid calibration, can be used to generate measured values.
The IDS Gate is excellently suited for starting a lab on its digitalization path, as it can be implemented easily and step by step.

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Any further questions?
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