Agenda

Working Group Sample Prep introduction

Scope definition

Unit Operation: Model for data structuring

D-SI: Standard format for measure values

Conclusion
WG Sample Prep: Members

- Reinhard Baumfalk, Sartorius (WG Lead)
- Pasi Kankaanpaa, Sartorius
- Thomas Schink, Sartorius
- Holger Linnerz, Mettler Toledo
- Gerald Hall, Agilent
- Heiko Fessnmayr, Agilent
- Hossein Arjomand, Thermo Fisher

- Matthew Fox, ALLOTROPE
- Christoph Schaub, Bayer
- Raghu Arrola, Astra Zeneca
- Wolfgang Colsmann, Osthus
- Helge Krieg, Osthus

... are still open for more
WG Sample Prep: Status

- Model for data definition finalized
- Review with ALLOTROPE Modelling group / Architects ongoing
- Prototypes for examination Unit Operation concept in preparation (Sartorius, Agilent)
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Sample Prep: some Impressions
(what do we understand talking about sample prep)
Sample Prep: Definition

Wikipedia:
In analytical chemistry, sample preparation refers to the ways in which a sample is treated prior to its analyses. Preparation is a very important step in most analytical techniques, because the techniques are often not responsive to the analyte in its in-situ form, or the results are distorted by interfering species. Sample preparation may involve dissolution, extraction, reaction with some chemical species, pulverizing, treatment with a chelating agent (e.g. EDTA), masking, filtering, dilution, sub-sampling or many other techniques. Treatment is done to prepare the sample into a form ready for analysis by specified analytical equipment.
Sample preparation could involve: crushing and dissolution, chemical digestion with acid or alkali, sample extraction, sample clean up and sample pre-concentration.

Allotrope WG:
Needed information to ensure completeness of analytical data (sample prep and analysis) and to improve quality of data analytics.

Source: https://en.wikipedia.org
Scope for sample prep WG

Sample analytics
Requirements for documentation: Stakeholder view

**Scientist**
- Reliability in analytical results
- Traceability of results
- Comparability of results

**Lab Manager**
- Execution quality
- Flexibility in protocol execution
- Lab work optimization

**Pharma Manufacturer**
- Development speed
- Efficiency

**Lab IT**
- Consistent, safe, secure data management
- Completeness of data
- Easy access to all collected data

**IT integrator**
- Easy to integrate all kind of lab equipment
- Buildup domain specific network & data structures

**Asset supplier**
- Provide easy to use lab solutions
- Establish new solutions to make lab work easier
- Ensure the proper use of assets
Challenges for Sample Prep workflow documentation

- Due to protocols with many steps the error propagation should be managed & documented
- Large variance of processes, low standardization
- Multiple manual steps without defined documentation methods
- Most often, the workflow is known on high level, not in single step details
- Variety to achieve same results by providing different subprocesses
- Error propagation after execution of many steps should be considered
- Due to protocols with many steps the error propagation should be managed & documented

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Sample Prep: WG concept

Sample Preparation for Analytic (e.g. HPLC, ...):

- Weigh sample
- Dilute sample
- Set pH value
- Create concentration series
- Filter samples

For a Lab scientist/technician this workflow is sufficient, gives on a high level enough information but:
- Each step consists of sub steps
- For execution of these steps different instruments, tooling, assets, ingredients are needed. These can differ from lab to lab, lab technician, stock, ...
- Execution of the steps and the sub steps are depending on the lab technician’s experience.
- Documentation of the actual execution is not done in most cases
Concept “Unit Operation” for elementary lab processes
Modelling elements for lab work

Sample Prep Workflow:
Consists of a sequence of elementary services (Unit Operations).
Defines and / or documents the executed process as a composition of Unit Operations.

Unit Operation:
a digital representation of an elementary lab process including data for
- workflow,
- used means (instruments & consumables),
- parameters
- achieved results
Unit Operation: Key benefits

- Sample prep workflow consists of a collection of Unit Operations, no additional detail on this level needed
- Workflow design and process documentation is based on lab perspective
- Provider of instruments and material to lab can provide Unit Operations to optimize the use of their products
- Structuring of data along services, not instruments
- Parameter and results are assigned to the service, not to the device
- Instruments mostly providing more than one workflow (application)
- Same structure for manual or instrument supported workflow can be used
- Flexibility is given for different types of instruments
- Lab automation can also be covered by the Unit Operation model
Use Case: Collecting UO data during execution

1. **Weigh sample**
   - Description
   - Parameter
   - Results

2. **Dilute sample**
   - Description
   - Parameter
   - Results

3. **Set pH value**
   - Description
   - Parameter
   - Results

4. **Create concentration series**
   - Description
   - Parameter
   - Results

5. **Filter samples**
   - Description
   - Parameter
   - Results
Use Case: Sample Prep in a managed lab

Unit Operation model could be a benefit of Lab IOT data architecture:

- Decentralized service structure
- Simple, flexible integration of lab components
- High quality data acquisition standards
- Flexible workflow design
- Full traceability of sample preparation work
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Conclusion
The definition of a standard for measure data in the digital world is essential for the exchange of metrological information in all fields of Information and Communication Technologies (ICT).

In terms of content, the format considers essential international metrology guidelines and standards.

Publications:
Universal format for transfer of metrological data via digital communications
- https://doi.org/10.5281/zenodo.3522631
- https://doi.org/10.5281/zenodo.3522074
Use Case for D-SI

User Interface

- metre, °C, bar
- decimal
- Ä, Ö, Ü, métra

Machine Interface

- only SI
- JSON
- XML
- Dig. Calib. Certificate

Unambiguous, efficient, easy to understand, exchangeable

User Interface

- feet, °F, Pa
- binary
- 公尺 [公尺]
Digitalization for measure data is global ...

- Contacts und cooperations in 2018
  - SmartCom
  - 04/2018
  - 06/2018
  - 11/2018
- 03/2018
Key Objectives

- **Digital SI Metadata Model (D-SI)**
  - transfer of metrological data via digital communications
  - atomic and extended models
  - SI units vs. non-SI

- **Digital Calibration Certificate (DCC)**
  - standards like ISO 17025
  - secure transfer
  - Structure (administrative and measurement data)

Draft Version published 04/2020
D-SI: Real data model

\[ Y = y [\text{SI}] \pm U_{95}(k) \text{ distribution UTC} \]

- **SI unit format**
- **VIM**
- **ISO 80000**
- **IEEE 754**
- **RFC 362 (UTF-8)**
- **ISO 8601**

Example XML:

```xml
<si:real>
  <si:value>2.34</si:value>
  <si:unit>\text{metre}</si:unit>
  <si:label>\text{length}</si:label>
  <si:dateTime>2018-11-16T12:30:01.67-01:00</si:dateTime>
</si:real>
```
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- Unit Operation concept for sample prep processes creates the opportunity
  - To bring up precision of analytical results
  - To improve the quality of data (metrology)
  - To enable data analytics

- Unit Operation concept defines a concept
  - To cover the workflow, including manual work,
  - Acquire more information than the acquisition of pure measure data given by the used instruments.
  - Gives a definition for modelling workflows

- Unit Operation gives especially the sample preparation the potential to get a link to IOT

- Sample Prep is 1st example for ADF as input and output format (build data chains)
  (IOT: “vertical & horizontal data exchange”)

- With the Digital-SI format definition for measure values
  - Gives an universal standard for measure values
    (compared to the well established SI unit definitions)
  - Simplifies the management of calibration certificates of instruments (see DCC / DSI projects) by defining a common standard
Thank you.