jwLIMS Special Samples

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1. Why *jw*LIMS Special Samples?

The module jwLIMS-Special samples™, which is integrated in SAP R/3™, is a tool for the logistics of quality assurance in the chemical industry. It can also be applied in the pharmaceutical industry and the food industry.

The following targets are supported:

1. **Management of all inspection orders that cannot be mapped in the SAP standard or the jwLIMS™.**

2. **Precise implementation of the processes for the particular user.**

2. Characterisation of the special samples

The inspection orders for special samples fall into a separate category. They fundamentally differ from the release samples, the end samples, the returns and the repeat inspections (cf. jwLIMS) of an intermediate product, a finished product, an accumulation/waste, a raw material or a commodity.

- The quantity is not taken into account.

- Inspection results are not transferred to the batch.

- The inspection plan is edited dynamically to the inspection order.

Fields of application for special samples:

Research samples

An inspection plan is not available. It can only be developed at the end of the research, just before the beginning of the production.

The lower and upper limits are not yet fixed. The same applies to the inspection methods. All fields need to be highly flexible. Numbers in normal representation or floating-point representation or texts for the input. Lower and upper limits are not yet fixed.

Environmental samples

A material number and a batch make no sense. An inspection plan is available due to legal requirements.

Workplace samples, concentration measurements and emission measurements are common environmental samples.
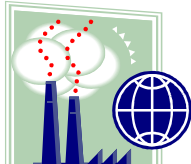
External samples

In *sporadic* orders no inspection plan, no material number and no batch is known. The inspection requirements are carried out in the external orders. In *regular* orders the relative master data have to be maintained.

Thus, an order LIMS can be implemented.

Additional inspections

Additional factory inspections for one or more characteristics that are not included in a standard inspection plan or a specification.

The characteristic to be inspected has to be selected from the amount of all present characteristics. The reference to the product (material number) and to the batch has to be guaranteed in order to make special releases or special blockings (even in terms of specifications). Furthermore total evaluations of the product have to be implemented.

Microbiology
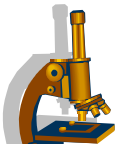
The inspection plan is not clearly defined. However, a part of the characteristics to be inspected, in which the total germ number often has to be determined, is defined.

Inspections of canteen meals and food samples are common applications.

Competitors

Inspection of the quality of competitor's products. In addition to the standard inspection plan, further characteristics have to be inspected. Product and batch have no connection to the implemented system.
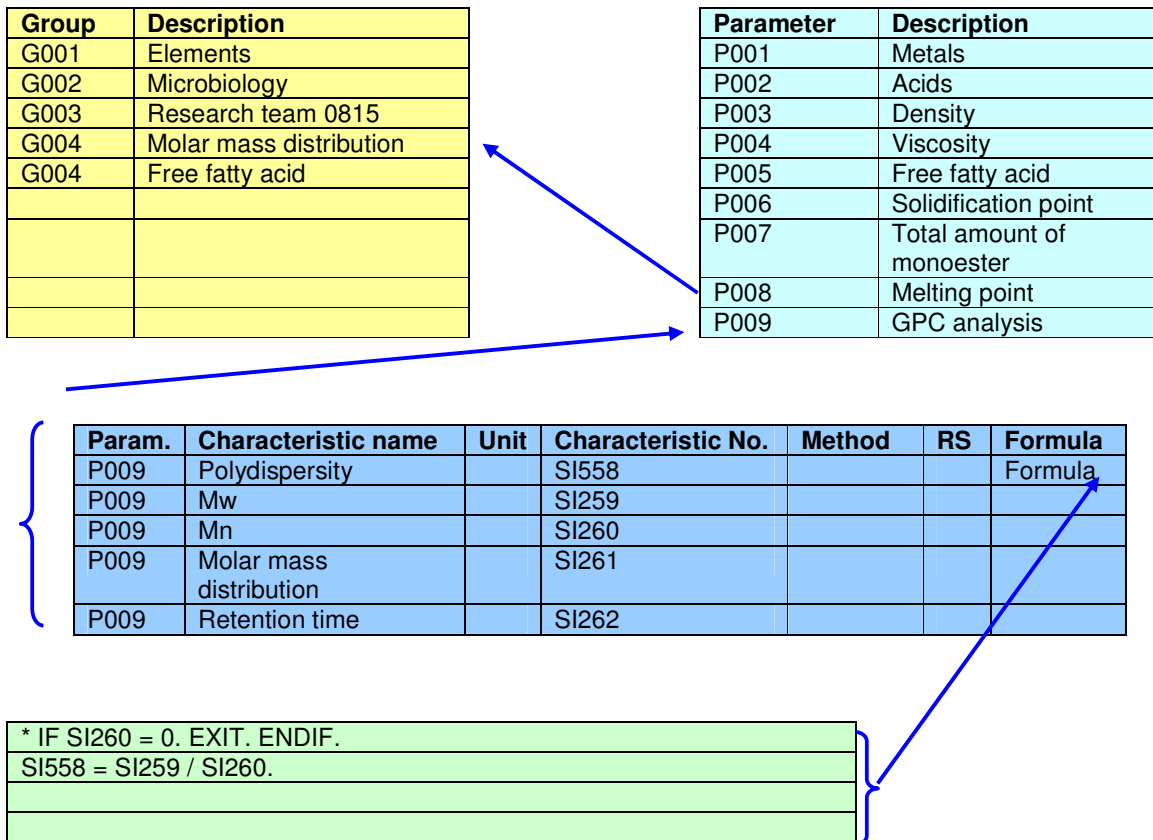
3. Functions

3.1 Master data

The master data are maintained in the SAP standard and in additional tables. Cf. jwLIMS-Master data.

In addition, editing was simplified for special samples because several characteristics often have to be selected from the total of all characteristics.
The characteristics can be arranged in groups with any definition, for example: groups of characteristics for the elements, microbiology, for a research team or the molar mass distribution.

This classification is usually too rough. Therefore parameters are assigned to the groups. The characteristics are then assigned to the parameters. Within a parameter formulas can be established to define determined characteristics. Determined characteristics are presented in the acquisition mask, but they cannot be changed there. For this reason a special maintenance transaction was implemented.

Simplified example

Group	Description
G001	Elements
G002	Microbiology
G003	Research team 0815
G004	Molar mass distribution
G004	Free fatty acid

Parameter	Description
P001	Metals
P002	Acids
P003	Density
P004	Viscosity
P005	Free fatty acid
P006	Solidification point
P007	Total amount of monoester
P008	Melting point
P009	GPC analysis

Param.	Characteristic name	Unit	Characteristic No.	Method	RS	Formula
P009	Polydispersity		SI558			Formula
P009	Mw		SI259			
P009	Mn		SI260			
P009	Molar mass distribution		SI261			
P009	Retention time		SI262			

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* IF SI260 = 0. EXIT. ENDIF.
SI558 = SI259 / SI260.
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The parameter P009 was assigned to group G004. Five characteristics were assigned to parameter P009. Characteristic SI558 is a formula characteristic. Of course, the characteristics used in the formula need to be quantitative characteristics. In the formula all valid ABAP/4 arithmetical operations and functions are permitted without limitations.

Several characteristics can be formula characteristics within one parameter. The random sampling for the acquisition of individual values can be deposited under RS (random sample size > 1).

This is one of many references to the R3 standard. Other fields such as laboratory, workplace, limits, unit, methods, method number were skipped deliberately.

3.2 Authorizations

Authorizations are deposited in the authorization concept. Due to the high requirements and the central basic maintenance of the LIMS, however, the program was upgraded. Thus, research samples can only be viewed from the particular laboratory / workplace. Laboratory / workplace are deposited in the authorization concept. Brightness control and blanking control of sensitive fields can be administered by each user. The key account managers have special rights such as the "manual completion" of an external sample.

3.3 Sample application

All sample applications for special samples are controlled by the inspection method – an SAP key deposited in the customizing. According to the set inspection method, different header information is demanded. Set inspection methods are:

- ZS01 Internal special samples
- ZS02 External special samples
- ZS03 Logistics special samples

Internal special samples have an internal customer who is automatically recommended by the system. Each user has a clear customer ID. Only if the customer works for several cost centers, the field cost center accepts input and the limited validation is implemented. Search assistance is available.

External special samples have header information which is deposited in the debtor's master data. This includes the customer, the key account manager and the customer's contact. The consistency of the key account manager (KAM) is inspected when issuing the inspection order because special rights are deposited due to the specific responsibility. The KAM is the only person to decide whether the inspection order is completed. Price information, date and laboratory are further fields.

Logistics special samples have a reference to jwLIMS via the batch.

The selection of an inspection plan from a list and input of text information into an SAP standard editor are standard header functions. Alternatively a sample application can be selected from a list of existing "similar" inspection orders. In this case, the fields sample generic term, sample description and sample identification are to be used. These fields and the sample ID form the second clear key. In the end the sample information fields such as sample drawing date, sample drawing time, sample type, sample drawing place or dangerous goods note can be filled. If a sample application is to be created several times, the appropriate option needs to be set.

There are three possibilities to enter the inspection characteristics dynamically:
- inspection plan (header function, link to SAP standard)
- parameter data file (cf. master data)
- individual characteristics (from the characteristics of the SAP standard)

All three possibilities can be combined arbitrarily. An inspection plan can also be left out or be replaced. Several parameters (even the same) can be selected or deleted. One characteristic can be entered several times as well. Individual values can only be acquired via the inspection plan or the parameters.

3.4 Registration

Registration is a necessary step. It means that the sample has physically arrived in the laboratory and that the determination of the characteristics can begin. Registration can be made manually or automatically, according to the setting in the leading laboratory. A sample accompanying booklet can be printed immediately or later.

3.5 Value acquisition

The value acquisition can be started via a working stock, a user menu or via direct transaction invocation.
The value acquisition is carried out via 4 registers as the presentation of all fields is confusing. It can be set which fields are shown in which register.

Simplified example for the register value acquisition

Characteristics	Value	Unit	S	L	Lower limit	Upper limit	Theor. value	Method
Polydispersity	0,5		2					
Mw	1		2					
Mn	2		2					
Molar mass distribution			1					
Retention time			1					

In the inspection order parameter P009 was selected. Polydispersity is determined. Therefore the field does not accept input. The formula can be presented.

The field S (status) indicates the status (1 = no value was entered, 2 = value was entered or determined, 3 SKIP: characteristic not measured).

The field L (limit) indicates a limit violation. Lower limit, upper limit and theoretical value can be entered. Suggested values can be deposited in the parameter. The unit and the inspection method can be suggested from the parameter.

In other inspection orders, for example, in the acquisition of individual values, the acquisition mask changes automatically. Furthermore the value acquisition of a characteristic is planned for several inspection orders.

Simplified example for the value acquisition of a characteristic in several inspection orders

Characteristic: Density   Unit: g/cm³ Method: Standard DIN   Temperature: 25°C

Sample ID	Sample description	Value	S	L	Lower limit	Upper limit	Theor. Wert
30000100	OB1 Kunde 1 CV11	**1,05**	2				
30000101	OB1 Kunde 1 CV12	**1,52**	2				
30000205	OB2 Intern 28 Prod 1		1				
30000300	OB3 Kunde 25 X25		1				

Further registers are designed for additional information, for prices and further changes.

In the *additional information* a long text is planned for each characteristic (not to be confused with the long text of the inspection order). Here information for the crude data reference can be deposited. In the analysis requirements room temperature, air humidity and other requirements can be recorded. Another text field is for additional comments. Here a free text is entered or a predefined text is adopted from a list. Again search assistance is available.

The *prices* are acquired only for the authorized laboratory; otherwise the price field is blank. Not all users have access to the prices. A price may only be entered after a value has been acquired. In case that a price is entered, the value may not be deleted. In case that the price for this characteristic has already been invoiced, the price cannot be changed anymore. Then the price fields do not accept input. Suggested values can be entered from a bill of quantities by means of search assistance. The suggested values can also be overwritten manually. Via another field a percentage discount or a surcharge for any additional costs can be granted.

When pressing ENTER the sum for the total order is indicated in the field "current price". In case that the sum exceeds the fixed price or the price limit, a warning is issued.

In the register *"further changes"* characteristics can be added, deleted or modified in the acquisition mask, which is carried out according to strict rules, especially when concerning the deletion of characteristics. Inspection method, unit, text field "Inspection for", laboratory and workplace are fields for modification.

Each field shows if input is possible and the kind of input. This can be indicated.

Characteristic attribute	Input	Comment
Formula	no	Quantitative formula characteristic. Calculated by the system when pressing ENTER if all operands have a value and a calculation is possible.
Normal	yes	Normal quantitative characteristic.
Value i	yes	Input of individual values for quantitative characteristic. i= 1,2,3, n as set in the random sampling. An individual value is never an operand for a formula characteristic.
Mean value	no	Mean value is always calculated automatically if input of individual values is demanded. The mean value always stands above the individual values.
Catalogue	yes	Selection set for a qualitative characteristic. Preferably the selection set is entered via the search assistance.
Free text	yes	Qualitative characteristic for which intentionally (function) no selection set was provided.

3.6 Further functions

■ Copy, change, present inspection order

The rights are limited. Only a user who is authorized for the selected inspection order is allowed to use this transaction. *One* of the following reading preferences has to be implemented

- universal right for all special samples
- authorization for the laboratory of the sample header
- authorization for at least one characteristic of the sample
- authorization for the cost center of the inspection order

When copying at least the sample description (3 fields) has to be modified, as this is the second clear ident of the sample. The sample ID is allocated automatically.

In case that the inspection order is already registered, only the header may be changed.

■ Print analysis results.
This function can be carried out during the value acquisition or as a separate transaction.

■ Accounting
Implements an individual accounting on the characteristics level, when the SAP standard is supposed to be dispensed with. The results are Excel lists. The add-on ensures that one characteristic can be invoiced only once. An accounting error can be corrected with a correction program.
Access is only restricted to the responsible user and his representative.

■ Sales
Two transactions are planned for sales.

- "Expected sales". Sales after the last accounting per key account manager, added up per laboratory and cost center, subdivisible according to orders of a debtor.

- "Achieved sales". Sales in a time interval per key account manager, added up per laboratory and cost center, subdivisible according to orders of a debtor.

■ Open characteristics per workplace. Print list for control purposes.

■ Chart (cf. jwLIMS)

4. Interaction with further jwProducts

The module *) **jw**LIMS-Special samples™ can be combined with the module **jw**LIMS™.

*) These modules (add-ons) utilize SAP R/3 workbench technologies and are written in the ABAP/4™ programming language and increasingly in Java™. The development yields SAP's best practices guidance to guarantee for stable applications which survive SAP release upgrades. The jwConsulting company exclusively used procedures which were designed for that purpose, such as BAPI components, batch inputs, user exits and customer name prefixes. Still, in order to prevent for obstructive redundancies, R/3 is and remains the master system in respect of the master data.

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