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EXPERT SYSTEM SUPPORTED INFORMATION AND MANAGEMENT SYSTEM FOR ANALYTICAL LABORATORIES

Abstract

The demand for high efficiency and short response time calls for the use of computer support in chemico-analytical laboratories.
This is usually achieved by laboratory information and management systems covering the three levels of analytical instrument automation, laboratory operation support and laboratory management.
The management component of the systems implemented up to now suffers from a lack of flexibility as far as unforeseen analytical investigations outside the laboratory routine work are concerned. Another drawback is the lack of adaptability with respect to structural changes in laboratory organization.
It can be eliminated by the application of expert system structures and methods for the implementation of this system level.
The ELAN laboratory information and management system has been developed on the basis of this concept.

Expertensystemgestütztes Informationssystem für die Laboranalytik

Zusammenfassung

Die Forderung nach hoher Effizienz und kurzen Antwortzeiten verlangt die Unterstützung von Computern in chemisch-analytischen Labors.
Dies wird gewöhnlich erreicht durch ein Laborinformations- und Management-system, das die Bereiche Laborautomation, Laborbetrieb und Labormanagement abdeckt.
Bei den bisher realisierten Systemen verfügt die Managementkomponente nur über eine eingeschränkte Flexibilität gegenüber Änderungen der Routine-analytik. Ein weiterer Nachteil ist die mangelhafte Adaptierbarkeit in bezug auf Änderungen in der Labororganisation.
Diese Einschränkungen können durch den Einsatz eines Expertensystems weit-gehend umgangen werden.
Auf der Basis dieses Konzepts wurde das ELAN-System entwickelt.

E L A N

Expert System Supported Information System for Analytical Laboratories.

ELAN is a knowledge based laboratory control and information system. It can be used for the planning, control and evaluation of the problems occuring in an analytical laboratory.

1. What Is the Difference Between ELAN and Other Laboratory Information Systems:

1.1 Conventional Systems:

Most of the laboratory information systems implemented up to now have an extensive functional scope on the laboratory operation level. Their laboratory management level, however, is more or less limited. Systems without this disposition level can only be used for data acquisition and management. The computer support potentials are not exploited to the full extent.

1.2 Systems With Management Function:

The problems resulting from the integration of a management level have not yet been solved satisfactorily:

- Usually, laboratory-specific management strategies are developed. They depend on the special objective as well as on the structure and the equipment of the laboratory. For laboratory-specific conception and implementation of the laboratory management components, a correspondingly high expenditure is required. In contrast to this, the modules of the laboratory operation level can be implemented in a more or less modular manner. Only structurization and parameterization are to be carried out in a laboratory-specific manner.
- Except for the few laboratories carrying out routine analytics only, laboratory management is very dynamic. The variety of orders placed is changed constantly. New analytical instruments and methods are applied and new process and safety regulations are introduced. This leads to permanent changes of the boundary conditions for the disposition in the laboratory. As a result, continuous adaptation of the strategies of the laboratory management level is required to meet the new requirements imposed and to make use of the experience gained.

In practice, however, this means continuous adaptation and modification of the application programs on this level. For this purpose, both application-specific know-how and the corresponding programming capacity have to be provided during service life on the system. Moreover, permanent modifications adversely affect the quality of the application software. It loses its original structure and, hence, becomes increasingly unreliable and unmaintainable.

To solve the problems mentioned above, the decision and planning functions of the laboratory management level can no longer be executed by conventional program system components, but rather have to be integrated into the laboratory information system as an expert system. In this system, the knowledge used as a basis for the management is stored and managed in a knowledge base (s. Fig. 1).

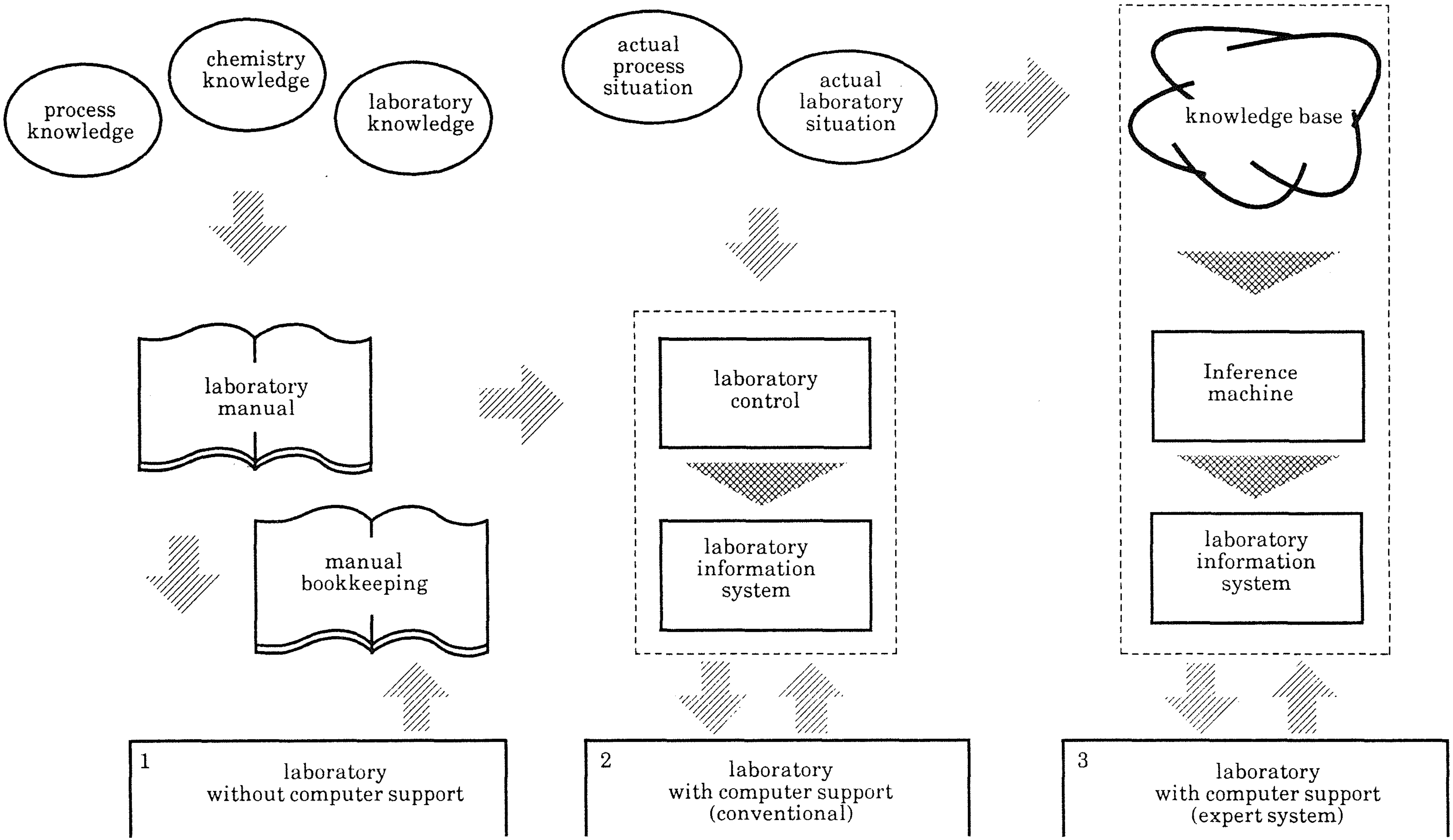


Fig. 1: Comparison of organizational structures

1: Laboratory Without Computer Support:

In a laboratory without computer support, organization is based on a standardized schema (often documented as a laboratory manual) according to which all analytical processes are controlled. This schema was specified by a laboratory/chemical expert on the basis of his knowledge and experience gained in the fields of chemistry, laboratory and process. Although standardization implies simplification, a loss of flexibility and efficiency can be noticed. Thus, the standardized schema can only be used for routine work in the laboratory. In exceptional cases, the laboratory expert has to interfere and processing is carried out outside the standardized schema.

2: Laboratory With Computer Support (Conventional):

In all conventional laboratory information systems implemented up to now, the standardization schema is modelled and used as a basis for the disposition functions. For this reason, these systems are not characterized by an increased flexibility.

3: Laboratory With Computer Support (Expert System):

This is not true for expert system supported systems. Instead of the standardized schema with its inherent drawbacks basic knowledge itself which originally had been used for the generation of the schema can be integrated into the system as a laboratory and process model. This step backwards from the "derived" (surface) knowledge to the "primary" (basic) knowledge enables the system to make disposition decisions on the same knowledge level as the laboratory/process expert. This means that flexibility with respect to non-routine requests is also the same.

1.3 Solution for LIMS With the Management Level:

The following program system components are obtained:

- System:

  The software system is embedded into the hardware and software environment, i.e., access mechanisms, interfaces with other software systems such as process information system or laboratory quality control and interfaces with the laboratory automata.

- Laboratory operation:

  The analysis is carried out. Samples are taken and analytical and intermediate results are determined. The user is informed about troubles arising (trouble report).

- Problem solution:

  Complete laboratory disposition is carried out and the results obtained are checked. The control standards are generated for the modules of the laboratory operation component.

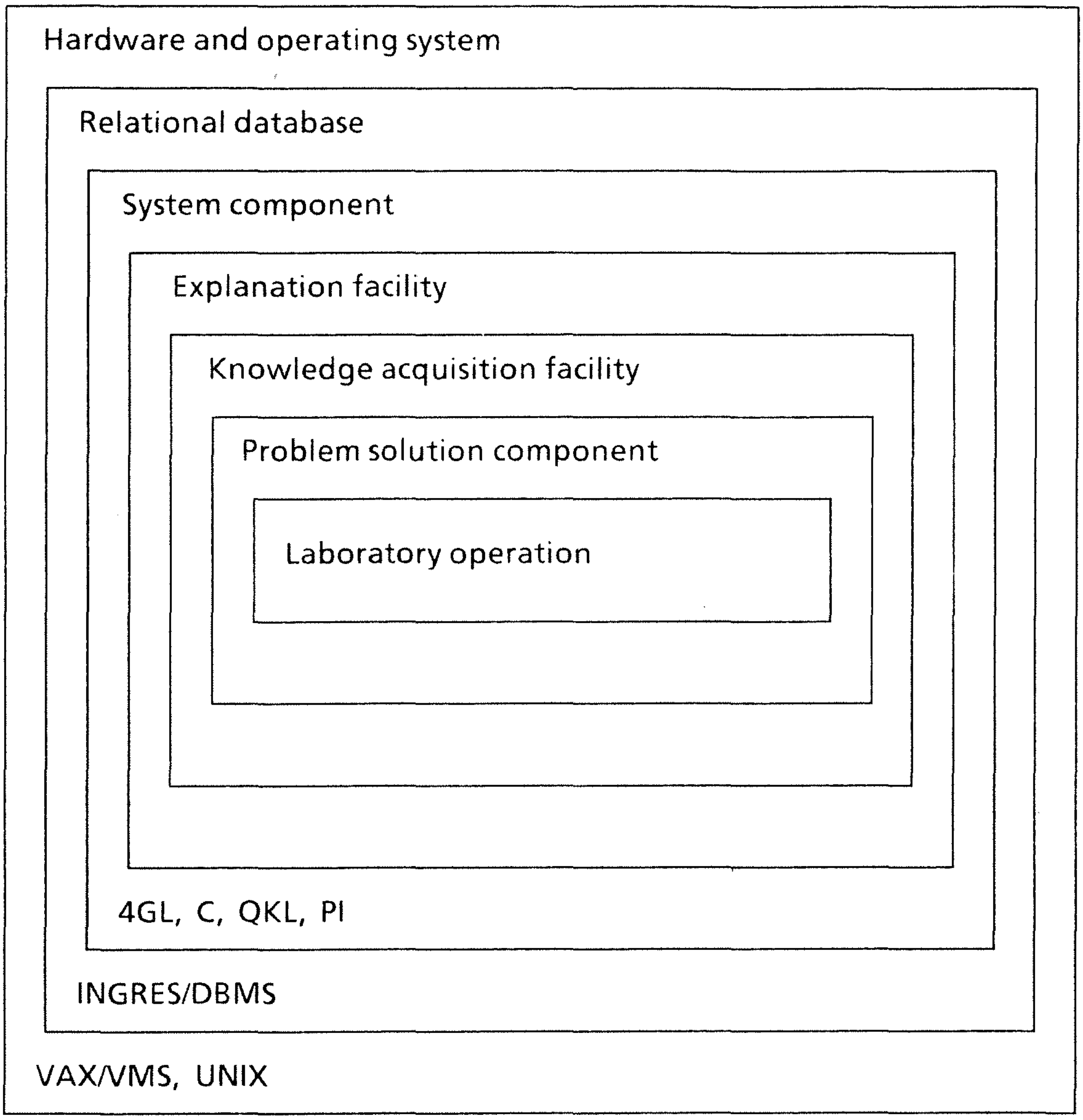
- Knowledge acquisition:

  The knowledge stored in the knowledge base is updated and modified. During system generation or maintenance, the other components do not need to be modified.

- Explanation:

  The user is enabled to reconstruct and control the individual steps of the respective problem solution process.

ELAN-Model



4GL = programming language of the fourth generation
QKL = quality control of the laboratory
PI = process information system

2. Structure of ELAN:

In a computer supported Laboratory information system three levels can be distinguished:

- Laboratory automation level

  This level mainly includes instrument-related functions which are generally controlled by means of microprocessors. The interfaces are provided by the system.

  Usually, this activity is performed by the system manager.

- Laboratory operation level

  The following functions are included:

  - Placing of orders
  - sampling
  - workstation management
  - acquisition, determination and acknowledgment of results
  - trouble report, etc.

  Usually, this activity is to be carried out by the laboratory chemist. These are procedural functions which comply with the sequences of activities in the laboratory.

- Laboratory management level

  Here, the following functions are included:

  - method selection
  - disposition of personnel and instruments
  - workstation disposition
  - check of results, etc.

  These are decision and disposition functions which usually are dealt with by the shift supervisor in the laboratory.

The ELAN structure is based on a hybrid system and consists of the following modules:

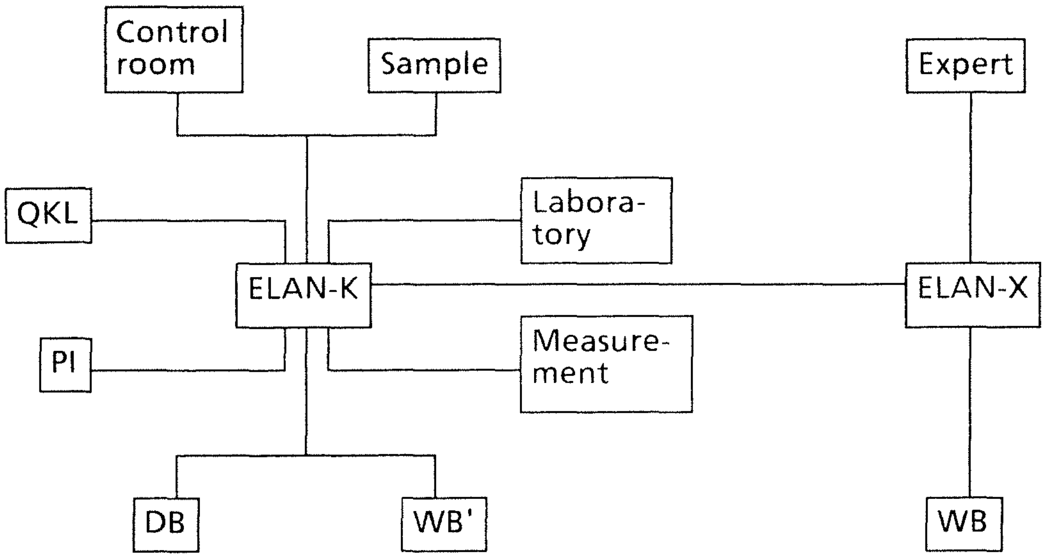
- ELAN-K, conventional system with management component limited to routine analytics

  laboratory automation level and laboratory operation level

  ELAN-X, expert system

  laboratory management level

This organizational structure enables both systems to be operated independently of each other. This means that during the introductory step, the conventional system can be generated and operated at first. Upon the completion of this step, the management level is taken over by the expert system in a second step.



DB = database
QKL = quality control
WB, WB' = knowledge base
PI = process information system

3. Most Important Properties of ELAN

The most important properties of ELAN can be described as follows:

- Flexible adaptation of ELAN to an existing laboratory and an existing laboratory organization;
- adaptability to structural changes in the laboratory organization when new analytical instruments and methods are introduced;
- flexibility as far as unforeseen orders for analyses outside routine analytical work are concerned;
- simple user interface, the control of which depends on the rights of access, analysis regulations, availability of instruments at the working place, actual situation of the working place and the hazard potential of the material to be investigated;
- maximum system independence of the computer and operating system, as the complete system is implemented in the relationally distributed INGRES database using 4GL OSL/SQL. Modules that cannot be implemented in SQL are available in 3GL PASCAL or C. INGRES is available in all common computer versions;
- use of an expert system in the management component.

4. Execution of Orders

The complete process of order execution can be devided into the following steps:

- Placing of orders

  The order is placed. The staff is informed about

  - The place of sampling,
  - the type of analysis desired,
  - the parameters to be measured and
  - the priority of the order.

- Derivation of the analytical methods

  The analytical methods to be applied are derived on the basis of

  - the knowledge on the chemical process of the place of sampling,
  - the knowledge on the actual state of the process,
  - the measured values required and
  - the concentrations and measurement ranges to be expected.

- Determination of the sample volumes and sampling

  The volume is obtained on the basis of the knowledge on the analytical methods derived.

- Workstation disposition and process control at the respective working places

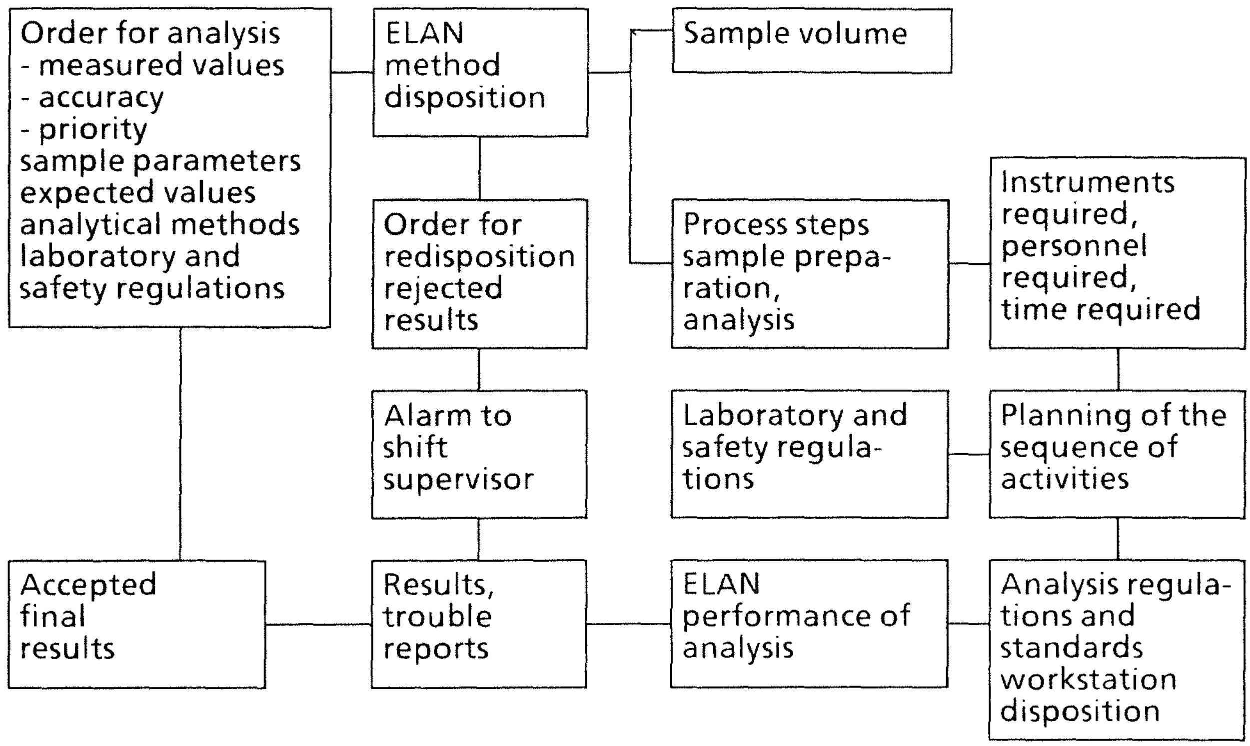
  In accordance with its priority, the order for analysis is placed into the respective queue of the working place (workstation) in the laboratory. Here, the following details are taken into account:

  - analysis regulations,
  - availability of istruments at the working place,
  - actual situation at the working place and
  - hazard potential of the material to be investigated.

- Determination, condensation and feedback of the results into the knowledge base

  The individual results are obtained in accordance with the analysis regulations. After the compilation of the results in accordance with the order placed, they are passed on to the laboratory management. Here, the order is checked and passed on to the customer. In case of failures, either redispositions of the process steps will be carried out or the complete order will be cancelled.

Disposition in the ELAN system:



In cooperation with the Institute for Data Processing in Technology (IDT) of the Karlsruhe Nuclear Research Center and the EPOS GmbH company, the ELAN system has been developed and conceived for use at the Karlsruhe reprocessing plant (WAK) (Fig.2).

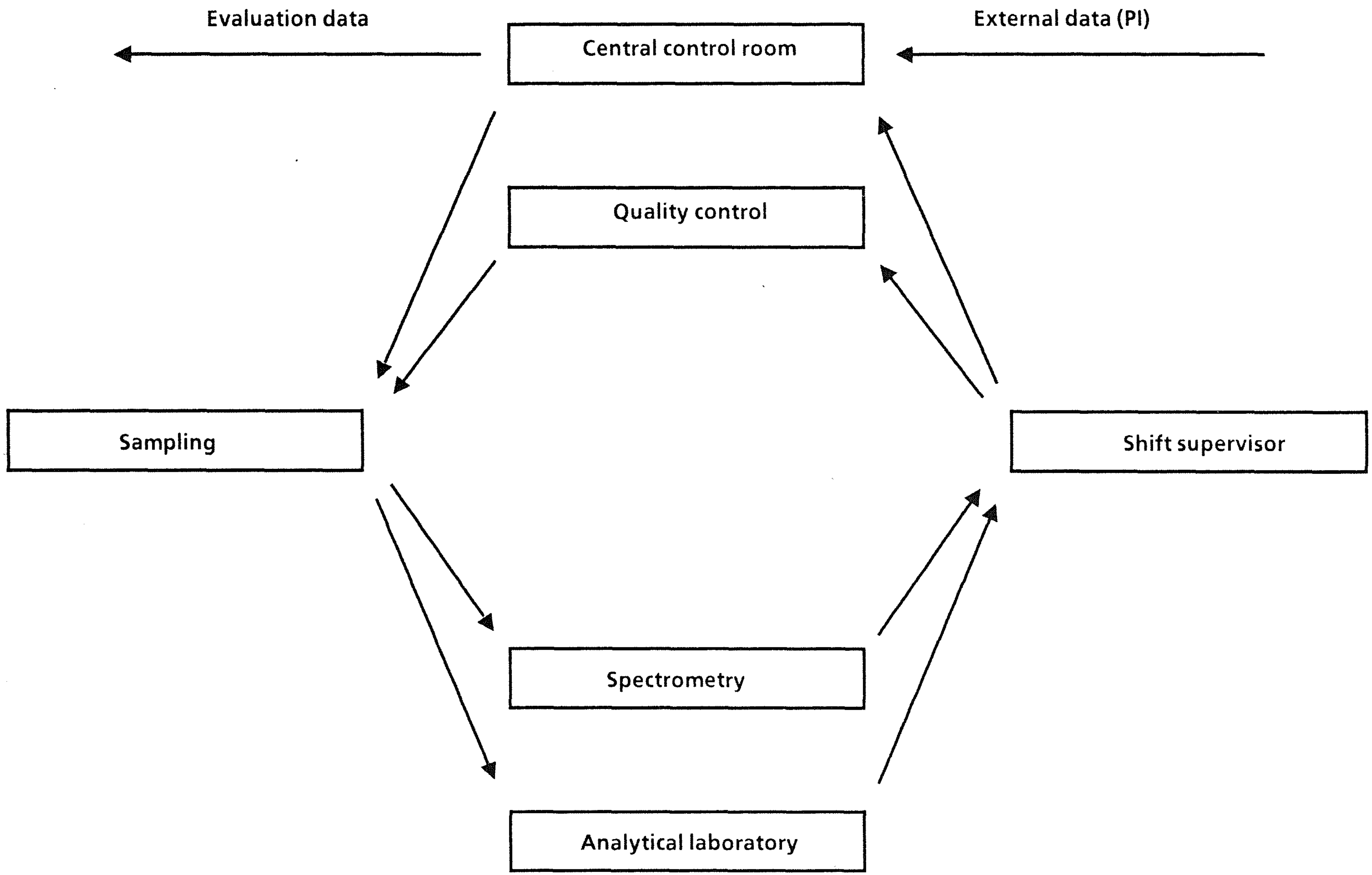


Fig. 2: Schematical representation of the WAK laboratory