Profiling of Software Requirements for the Pharmaceutical Enterprise Manufacturing Execution System

Vyacheslav Kharchenko, Oleksandr Gordieiev and Alina Fedoseeva

Abstract This chapter is devoted to analysis of existing Pharmaceutical Enterprise (PE) Manufacturing Execution System (MES) requirements. A special technique grounded on so-called Semantic Facet-Hierarchical Structures (SFHS) is suggested for the requirements profiling, development of general and particular PE MES requirements profiles taking into account software requirements of ISO/IEC 25010 "Systems and software—Systems and software Quality Requirements and Evaluation (SQuaRE)—System and software quality models" and GAMP "Good Automated Manufacturing Practice" standards. The chapter has the following structure: the Sect. 1 introduces into problem, the Sect. 2 describes features of PE and MES and corresponding standards, the Sect. 3 is dedicated to the SFHS-based technique analysis, the Sect. 4 presents case study and last one concludes and discusses future works.

1 Introduction

The modern society makes high requirements to computer-based systems and software in pharmaceutical enterprise. Thus the technological process of drugs production is closely related with patients risks, special attention should be to profiling of the manufacturing execution system requirements. Manufacturing execution system (MES)—specialized software used in technological process of drugs production.

V. Kharchenko (✉)
National Aerospace University "KhAI", 17 Chkalova Street, Kharkiv, Ukraine
e-mail: V.Kharchenko@khai.edu

O. Gordieiev
University of Banking of the National Bank of Ukraine, 1 Andriyvska Street, Kyiv, Ukraine
e-mail: alex.gordeyev@gmail.com

A. Fedoseeva
National University of Pharmacy, 53 Pushkinskaya Street, Kharkiv, Ukraine
e-mail: fedosaa@ukr.net

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There are serious requirements to reliability and safety of the instrumentation and control systems (I&Cs) and MESs as a specific type of such systems for pharmaceutical enterprise. Pharmaceutical enterprise (PE) is an industrial enterprise for drugs production. International industry software products such as Sparta Systems' TrackWise Enterprise Quality Management Software, AssurX, MARG and others, guarantee support the workflow management, tracking and regulatory reporting for all critical technological operations in process of drugs production [1–3]. Drugs—medicinal form in prepackaged, packaged and marked form according to the requirements for normative-technical documentation with the specified shelf life.

Applications of MESs are regulated by industrial standards ANSI/ISA88 and ANSI/ISA95. They define the models for batch process control [4] and the models of manufacturing operations management [5].

MESA [6] describes typical functions for PE, which covers all the operations of technological processes of drugs production. Designing of PE MES should be conducted by comprehensive assessing the quality and security of software [7, 8].

This chapter is devoted to analysis of existing PE MES requirements. A special technique grounded on so-called Semantic Facet-Hierarchical Structures (SFHS) is suggested for the requirements profiling, development of general and particular PE MES requirements profiles. The chapter has the following structure: the Sect. 2 describes features of PE and MES and corresponding standards, the Sect. 3 is dedicated to the SFHS-based technique analysis, the Sect. 4 presents case study and last one concludes and discusses future works.

2 An Analysis of Pharmaceutical Enterprise MES Related Standards

2.1 Features of PE MES

Nowadays more and more attention is given to application information technologies in PE. This is primarily due to the development of technological possibilities of pharmaceutical branch and also using of specialized software during technological process of drugs production.

These factors lead to the need to develop normative profiles for PE software. The software applied in PE domain should be aimed at reducing the negative effects for patients because of the failure or wrong usage of the software. The pharmaceutical industry faces the task of meeting all FDA [9] regulatory compliance requirements.

The technological process of drugs refers to:

- process-costing manufacturing type is sequence of technological stages (operations) each of which cannot be interrupted at any moment. PE are usually produced some accompanying or by-products besides drugs. Some technological stages (operations) in drugs manufacturing can be repeated recursively;

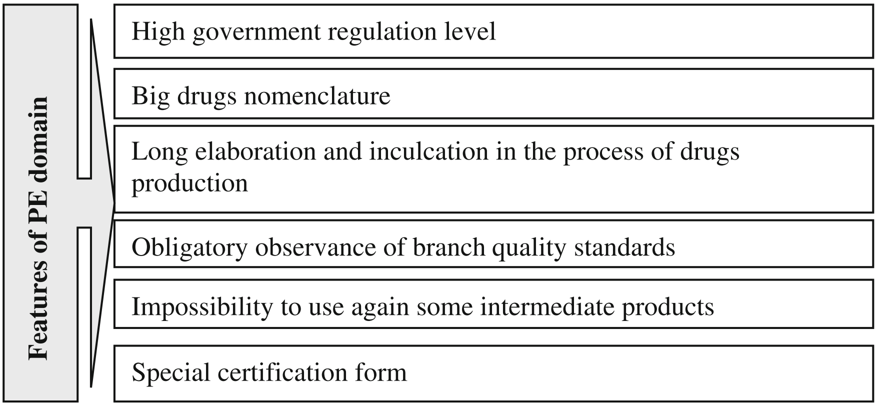


Fig. 1 Features of PE domain

- batch manufacturing type is application of thousands of recipes, ten thousands components in technological process of drugs, whose interaction is necessary to monitor (separately and ready-made drugs). Special recipes in a small amount are often used.

The technological process of drugs production must be implanted according to the technological regulation of drugs production and GMP rules.

Features of PE domain represented at Fig. 1.

MES for PE embody:

- organization and detail realization electronic document flow in PE;
- tools to control the quality of technological stage, technological operation and drugs or semi-manufactured goods. Technological stage (TS) is a complex of technological operations resulting in the information of intermediate product (at the end-product final step), which is determinate quantitatively and characterized by quality. Technological operation (TO) is a part of the technological process of drugs links one of the using equipment;
- control of industrial stocks and batches output;
- confirmation of drugs quality with electronic passport of drugs batch record, which contains information about technological process of drugs, including the data about operators and used materials. Electronic passport of drugs batch record (EBR) is an information about technological process including operation and used RM data;
- validation and revalidation of technological process of drugs production;
- optimization of technological process of drugs production.

The most important principle of MES project is modularity (Fig. 2), because the technological process of drugs production refers to Process-Costing manufacturing type.

For the correct and safe functioning of software in the critical PE MES it is required to analyze the existing international normative documents (standards, guidelines,

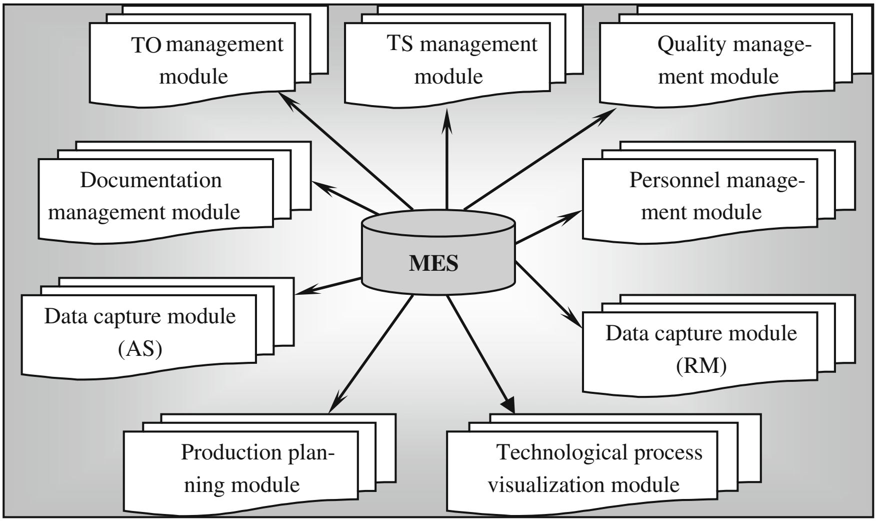


Fig. 2 Modular structure MES for PE

directives and technical reports) in all domains related to the technological processes of drugs production.

A lot of normative documents governing the technological process of drugs production with using special software can be divided into two groups: pharmaceutical enterprise standards and software engineering standards. The first group of standards includes regulations under which the technological process of drugs production, validation, revalidation and guaranteeing drugs quality are carried out.

The second group of standards includes regulations under which development, inculcation and accompaniment software processes are carried out. Today these two groups of standards are separately, but there is a need for general profile standards creation, which should be followed in technological process of drugs production in PE with MES.

2.2 PE MES Standards

MES development for PE is regulated by normative acts of MESA International (Manufacturing Enterprise Solutions Association), and also of standards international Society of Automation (ISA) [10]: ISA S95 "Enterprise Control System Integration" and ISA S88 "General and Site Recipe Models and Representation". MES standards were developed with the participation of leading automation systems manufacturers (Siemens, Rockwell Automation, Schneider Electric) and IT-companies (IBM, Oracle, SAP AG).

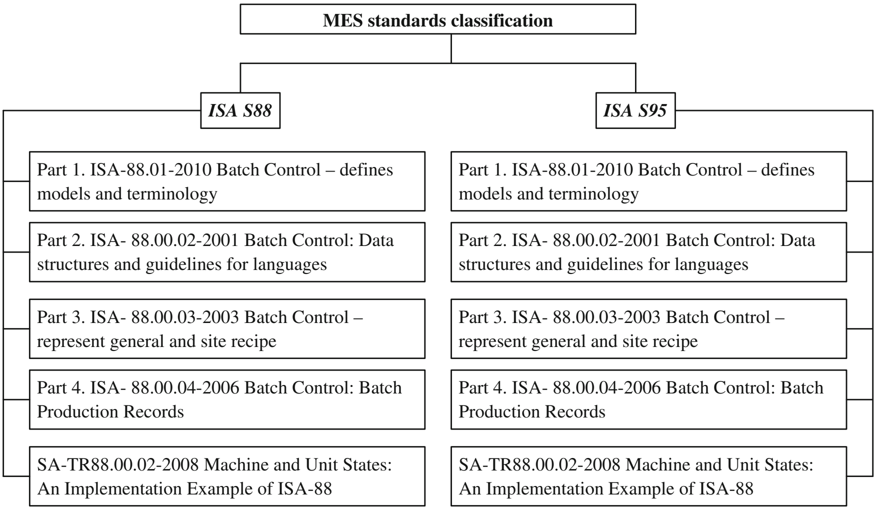


Fig. 3 MES standards classification

ISA S88 and ISA95 standards describe MES components development. Special attention in these standards is paid implementation features of the technological processes at enterprises.

According the specifications of ISA S95 standard the pharmaceutically relevant data are to be handled by the PE MES. ISA S88 standard contains models and terminology for controlling batch processes in PE. The standards differ in terms of their purpose, which means manufacturing companies will increasingly make use of both standards.

Pharmaceutical enterprise standards and software engineering standards MES standards classification is represented on Figs. 3 and 4. All PE standards are divided into groups. Each group consists of the main categorized standards: Quality

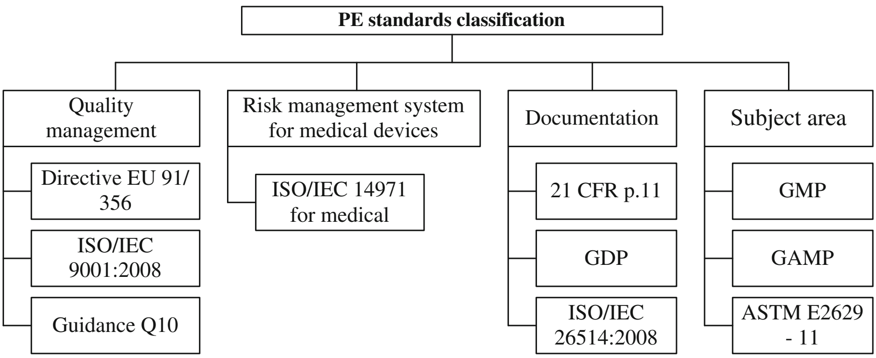


Fig. 4 PE standards classification

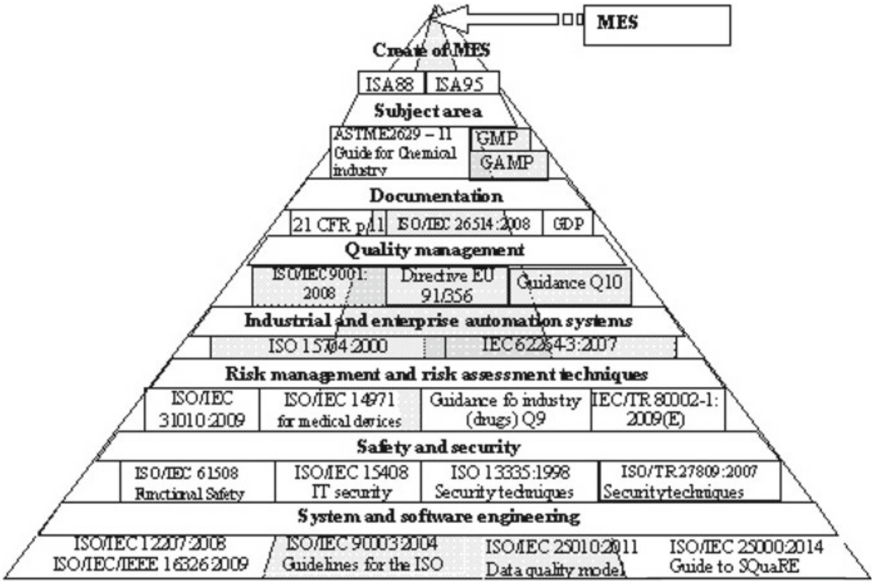


Fig. 5 Profile forming base for PE MES

management, Risk management system for medical devices, Documentation and Subject area. Each category corresponds to main requirements and guidelines.

2.3 Profile-Forming Base for PE MES

High-quality PE MES development requires a thorough analysis of the normative base of branches such as pharmaceutical manufacturing, validation of automated system in pharmaceutical enterprise, system and software engineering, documentation, risk management and assessment techniques. There are its own regulatory acts in each of these brunches.

International standards, guidelines, directives and technical reports, selected on the basis of the criteria [11] and listed above brunches were collected into profile-forming standards base. Figure 5 presents profile-forming base for PE MES.

3 SFHS-Based Technique for the Requirements Profiling

To develop MES software profile the standard requirements should be analyzed, selected and added as needed taking into account features of PE. For that SFHS-based technique is used.

3.1 Taxonomy Terms

Connections between concepts and represent in the facet-hierarchical structure form have been established (Fig. 6). Classification attribute identified by a number, and taxons identified by two numbers: the first is the number of classification attribute, and the second is the number of taxons.

Depending on the base (2) three types of ordering have been selected: the systematization of discrete (classification 2.1), continuous (grouping, 2.2) and self-organizing or procedurally interacting (clustering 2.3) of objects.

Classification is twofold. It is expressed in the approach to the classification of objects (3). There are two approaches to classification: taxonomic (taxonomy) (3.1), which is based on the decomposition of objects into classes, is characterized by more or less resemblance classification sets; meronomic (meronomy) (3.2) is based on the partition of objects into parts that have some common attribute (Fig. 6).

Following types of taxonomic structures (4) have been selected: hierarchical (4.1), a facet (4.2), facet-hierarchical (4.3) (mixed species), the matrix (4.4), descriptive (4.5). Degenerate cases of topologies are descriptive when difficult to determine of objects topology and matrix—when the topology is complex. The following operations for taxonomic structure (5) are defined:

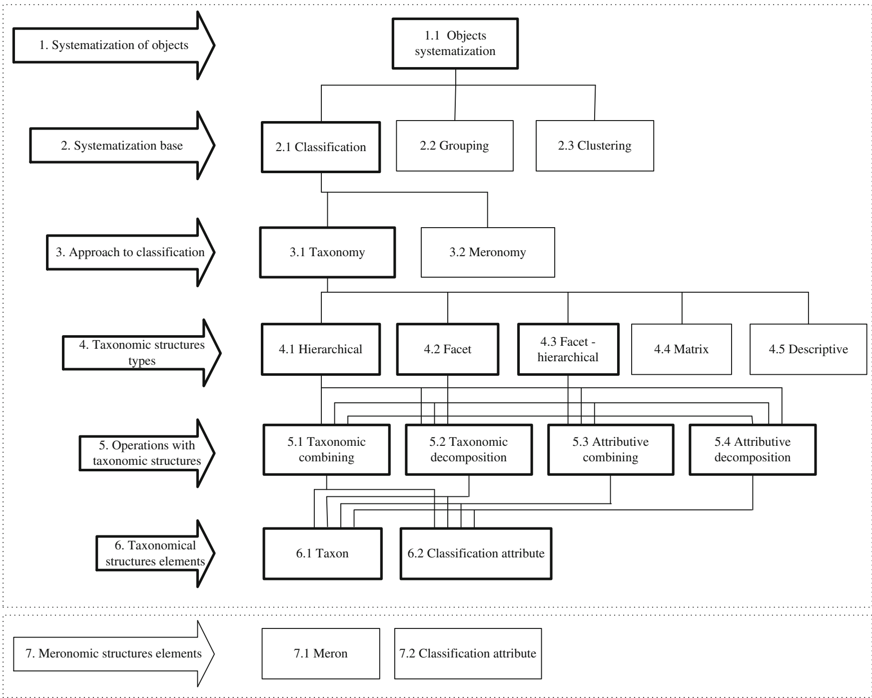


Fig. 6 Definitions facet-hierarchical structure

- taxonomic combining is combining of two taxonomic structures in an immutable set of classification attributes (combining in width) (5.1);
- taxonomic decomposition is partition on the basis of establishing equivalence between the elements of the taxon sets (T) and the choice criteria (C) (5.2);
- attributive combining is combining of two taxonomic structures at an increase of elements in set of classification attributes (5.3);
- attributive decomposition is decomposition of taxonomic structure on basis of establishment of equivalents between A and C (5.4).

Taxonomy is forming of external system out of objects. Meronomy represents them as internal structures. Taxonomic structure consists of (6) taxons (6.1) and classification attributes (6.2). Meronomic structure consists of merons (7.1) and classification attributes (7.2). Taxon is a set of objects, which are combined by some general classification attribute. Meron is a set of parts, belonging to these objects which have the same general classification attribute.

This work is oriented on formal operations with discrete objects. In this connection in future will consider one from systematization types—classification (taxonomy).

3.2 Variants of Taxonomic Structures

Taxonomic structures are represented by two variants of description: set-theoretic and set-matrix Taxonomic structure is set, consisting of three elements: $S\,\{\mathrm{A}, \mathrm{T}, \Psi\}$, where A—a set of classification attributes $A = \{A_i\}_{i=1}^{n}$; T—a set of taxons $T = \{t_i\}_{i=1}^{n}$; Ψ—relationship between elements $A_i \in A$ и $T_i \in T$, $A\Psi T$.

If the sequence of taxons or classification attributes is important, then this ordered set or tuple (marked as $\langle \ldots \rangle$), otherwise, taxons or classification attributes in taxonomic structures is unordered set usually (marked as $\{\ldots\}$). Taxons are unordered set, but for classification attributes sequence is important. To represent hierarchical structures ($\mathrm{S_H}$) we should use the following record: $\mathrm{S_H} = \{\mathrm{A_H}, \mathrm{T_H}, \Psi_{\mathrm{H}}\}$, where $\mathrm{A_H}$—a set of classification attributes in hierarchical structure; $\mathrm{T_H}$—a set of taxons in hierarchical structure; Ψ_{H}—relationship between elements of sets $\mathrm{T_H}$ and $\mathrm{A_H}$, in which connection is:

- $\mathrm{A_H} = \langle \mathrm{A_{Hi}} \rangle_{i=1}^{\mathrm{n}}$—a set (tuple) of classification attributes in hierarchical structure;
- $\mathrm{T_H} = \left\langle \ldots \left\langle \mathrm{t_{ij\ldots k}} \right\rangle \ldots \right\rangle$—a set (tuple) of taxons in hierarchical structure—inserted tuples, which provide possibility of description of subordination hierarchies;
- $\Delta T = \langle t_i \rangle$—subset (tuple) of taxons in hierarchical structure, which appropriate to classification attribute;
- $\Psi : \forall \mathrm{A_{Ii}} \leftrightarrow \Delta T_{Ii} \subset T_I$—relation between taxonomic classification attributes and a variety of taxons in a hierarchical structure.

To represent the facet structures ($\mathrm{S_F}$) we should use the following record: $\mathrm{S_F} = \{\mathrm{A_F}, \mathrm{T_F}, \Psi_{\mathrm{F}}\}$, where $\mathrm{A_F}$—a set of classification attributes in facet structure; $\mathrm{T_F}$—a set of taxons in facet structure; Ψ_F—relation between elements of sets T_F and A_F, in which connection is:

- $A_F = \{A_{Fi}\}_{i=1}^{n}$—a set of classification attributes in facet structure;
- $T_F = \bigcup_{i=1}^{n} \Delta T_{Fi}$—a set of taxons in facet structure, which consists of combination of each subset ΔT_F, corresponding to classification attribute (facet row);
- $\Delta T_{Fi} = \{t_{ij}\}_{j=1}^{n_i}$—a set of taxons, corresponding to classification attribute (facet row);
- $\Delta T_{Fi} \cap \Delta T_{Fj} =$—taxons subset, corresponding to different disjoint classification attributes (facet rows);
- $\Psi : \forall A_{Fi} \leftrightarrow \Delta T_{Fi} \subset T_F$—relation between taxonomic attributes and set of taxons in facet structure.

Set-matrix description of taxonomic structure represents the set of classification attributes (A) and the set of taxons (T). The relations between elements of these sets are represented by contiguity and compliance matrixes. Contiguity matrix for hierarchical structures is needed to represent logical relations between elements of set T, i.e. for description of topology (logical relations between taxons). The compliance matrix is used to for represent the compliance between elements of sets T and A. Example of representing hierarchical structures according to the model of description is depicted on Fig. 7.

Hierarchical structure (Fig. 7), consisted of sets $A = \{A_1, A_2, A_3\}$ and $T = \{T_{1.1}, T_{2.1}, T_{2.2}, T_{2.3}, T_{3.1}, T_{3.2}, T_{3.3}, T_{3.4}, T_{3.5}\}$ in the form of the contiguity matrix (Table 1) and the compliance matrix (Table 2) have been represented. The contiguity matrix is formed as following: "one" is an equivalent of logical relation between taxons, "zero" its absence. Compliance matrix formed as follows: "one" is compliance taxon with classification attribute in hierarchical structure, "zero" if compliance is absence.

For facet structures the compliance of elements T and A is determined the compliance matrix only, because logical relations of elements are absent in set T (Fig. 8). The facet structure (Fig. 8), consisted of sets $A = \{A_1, A_2, A_3\}$ and $T = \{T_{1.1}, T_{1.2},$

Fig. 7 Hierarchical structure

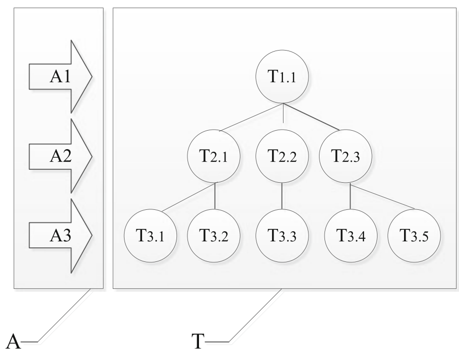


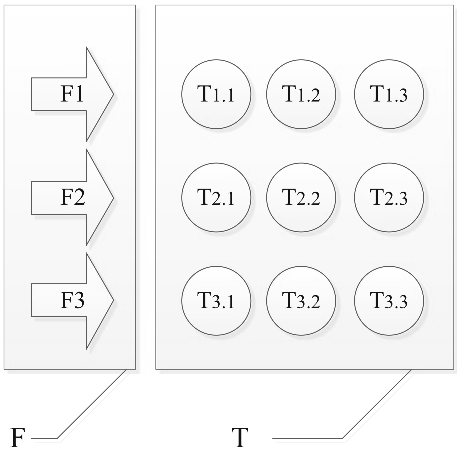
Table 1 Contiguity matrix

	$T_{1.1}$	$T_{2.1}$	$T_{2.2}$	$T_{2.3}$	$T_{3.1}$	$T_{3.2}$	$T_{3.3}$	$T_{3.4}$	$T_{3.5}$
$T_{1.1}$	0	1	1	1	0	0	0	0	0
$T_{2.1}$	1	0	0	0	1	1	0	0	0
$T_{2.2}$	1	0	0	0	0	0	1	0	0
$T_{2.3}$	1	0	0	0	0	0	0	1	1
$T_{3.1}$	0	1	0	0	0	0	0	0	0
$T_{3.2}$	0	1	0	0	0	0	0	0	0
$T_{3.3}$	0	0	1	0	0	0	0	0	0
$T_{3.4}$	0	0	0	1	0	0	0	0	0
$T_{3.5}$	0	0	0	1	0	0	0	0	0

Table 2 Contiguity matrix

	$T_{1.1}$	$T_{2.1}$	$T_{2.2}$	$T_{2.3}$	$T_{3.1}$	$T_{3.2}$	$T_{3.3}$	$T_{3.4}$	$T_{3.5}$
$A(F)_1$	1	0	0	0	0	0	0	0	0
$A(F)_2$	0	1	1	1	0	0	0	0	0
$A(F)_3$	1	0	0	0	1	1	1	1	1

Fig. 8 Facet structure



$T_{1.3}$, $T_{2.1}$, $T_{2.2}$, $T_{2.3}$, $T_{3.1}$, $T_{3.2}$, $T_{3.3}\}$ in the form of compliance matrix has been represented. It is identical to compliance matrix for hierarchical structure.

3.3 Operation of Combining

The basis of operation of combining is formation of the generalized taxonomic structure of original structures. The operation of combining consists of combining elements of sets T and A together.

To combine taxonomic structures it was suggested to use the following logical operations: $\cup$—combining of sets; $\cap$—intersection of sets; $\subset$—strict inclusion of one set into another; $\vec{\cup}$—taxonomic combining of taxons sets; $\cup\downarrow$—attributive combining of taxons sets; $\cup_{FHS}$—combining hierarchies into facet- hierarchical structure. The operations $\cup_{FHS}$, $\cup\downarrow$, $\vec{\cup}$ were introduced in first for the best representation variants of taxonomic structure combining.

Taxonomic combining types for hierarchical structure have been considered:

1. Taxonomic combining for hierarchical structures consists of combination of elements of taxonomic sets ($T = T_1 \vec{\cup} T_2$) , the set of attribute must remain unchanged ($A = A_1$). In which the connection combined with a set of taxons can be without intersection of elements ($T_1 \cap T_2 = \varnothing$) or with intersection of elements ($T_1 \cap T_2 \neq \varnothing$) (Fig. 9a).
2. Attributive combining of hierarchical structures consists of combination of taxons sets elements ($T = T_1 \cup\downarrow T_2$) and classification attributes elements sets ($A = A_1 \cup A_2$). In which the connection between combination of set of taxonomic classification attributes can be without intersection of elements ($T_1 \cap T_2 = \varnothing$, $A_1 \cap A_2 = \varnothing$) or with intersection of elements ($T_1 \cap T_2 \neq \varnothing$, $A_1 \cap A_2 \neq \varnothing$) (Fig. 9b).
3. Combining of hierarchical structures to facet-hierarchical structure. It is degenerated variant of combining. It is a case when the establishment of relations is impossible between sets A and T. Combining of hierarchical structures is realized due to the formation of two facet structures. Each taxonomic structure will be separated by the facet structure. In result each hierarchical structure will be separated facet structure.

The next considered types of taxonomic combining operations for facet structures are:

1. Taxonomic combination for facet structures consists of combining of elements of taxonomic sets ($T = T_1 \vec{\cup} T_2$) , set of attribute must remain unchanged ($F = F_1$). In which the connection of combination of set of taxons can be without intersection of elements ($T_1 \cap T_2 = \varnothing$) or with intersection of elements ($T_1 \cap T_2 \neq \varnothing$) (Fig. 10a).
2. Attributive combining of facet structures consists of combining the taxons sets elements ($T = T_1 \cup\downarrow T_2$) and sets of classification attributes elements ($A = F_1 \cup F_2$). Combining of set of taxonomic classification attributes can be realized without intersection of elements ($T_1 \cap T_2 = \varnothing, F_1 \cap F_2 = \varnothing$) or with intersection of elements ($T_1 \cap T_2 \neq \varnothing$, $F_1 \cap F_2 \neq \varnothing$) (Fig. 10b).

3.4 Forming of Sets of Variants Taxonomic Structures Combine

Forming of set of variants combining of taxonomic structures is developed on the basis of analysis compliance of logical operations. As a result of analysis the

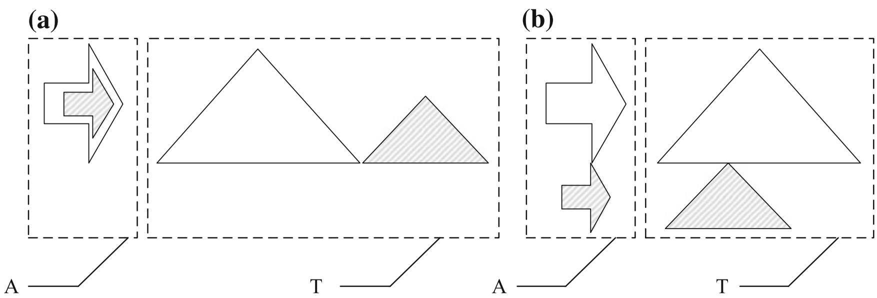


Fig. 9 Schematic representation of combining operations types for hierarchical structures

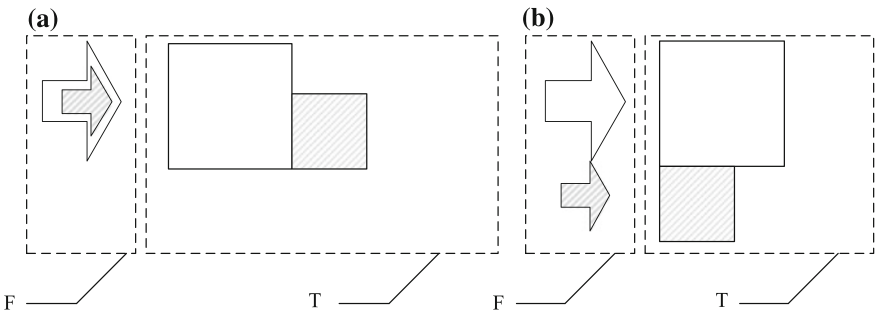


Fig. 10 Schematic representation of combining operations types for facet structures

taxonomic structures are determined by the following elements of operation of combining: $\overrightarrow{\cup}$—taxonomic combining; $\cup\downarrow$—attributive combining; $\cup_{FHS}$—combining in FHS; $T_1 \cap T_2$—intersection of taxons sets; $A_1 \cap A_2$—intersection of classification attributes.

The combinations of these elements are defined as a set of variants of combining taxonomic structures. In result of simple running over of elements we received full set of variants of combining taxonomic structures.

Two following additional variants of taxonomic structures combination exist: combination of hierarchical structures with inclusion of taxons set and with equality of taxons set. Description of variants of combining for hierarchical structures (Table 3) and for facet structures (Table 4) have been determined. Variants of combining for hierarchical structures are conceptually represented on Fig. 11 and for facet hierarchical structures are conceptually represented on Fig. 12.

Table 3 Formal description of hierarchical structures combined variants

1	Taxonomic combining of hierarchical structures without intersection of taxons sets (Fig. 11a) $\begin{cases} A = A_1; \\ T = T_1 \vec{\cup} T_2, T_1 \cap T_2 = \varnothing. \end{cases}$	(2.1)	2	Taxonomic combining of hierarchical structures with intersection of taxons sets (Fig. 11b) $\begin{cases} A = A_1; \\ T = T_1 \vec{\cup} T_2, T_1 \cap T_2 \neq \varnothing. \end{cases}$	(2.2)
3	Attributive combining of hierarchical structures without intersection of taxons sets and with intersection of hierarchies attributes (Fig. 11c) $\begin{cases} A = A_1 \cup A_2, A_1 \cap A_2 \neq \varnothing; \\ T = T_1 \cup \downarrow T_2, T_1 \cap T_2 = \varnothing. \end{cases}$	(2.3)	4	Attributive combining of hierarchical structures without intersection of taxons sets and without intersection of hierarchies attributes (Fig. 11d) $\begin{cases} A = A_1 \cup A_2, A_1 \cap A_2 = \varnothing; \\ T = T_1 \cup \downarrow T_2, T_1 \cap T_2 = \varnothing. \end{cases}$	(2.4)
5	Attributive combining of hierarchical structures with intersection of taxons sets (Fig. 11e) $\begin{cases} A = A_1 \cup A_2, A_1 \cap A_2 \neq \varnothing; \\ T = T_1 \cup \downarrow T_2, T_1 \cap T_2 \neq \varnothing. \end{cases}$	(2.5)	6	Combining of hierarchical structures with inclusion of taxons sets (Fig. 11f) $\begin{cases} A = A_1; \\ T = T_1. \end{cases}$	(2.6)
7	Combining of hierarchical structures with equality of taxons sets (Fig. 11j) $\begin{cases} A = A_1 = A_2; \\ T = T_1 = T_2. \end{cases}$	(2.7)	8	Combining of hierarchical structures in facet-hierarchical structure (Fig. 11k) $\begin{cases} A = A_1 \cup_{FHS} A_2, A_1 \cap A_2 = \varnothing; \\ T = T_1 \cup_{FHS} T_2, T_1 \cap T_2 = \varnothing. \end{cases}$	(2.8)
9	Taxonomic combining and attributive combining of hierarchical structures with intersection of taxons sets (Fig. 11l) $\begin{cases} A = A_1 \cup A_2, A_1 \cap A_2 \neq \varnothing; \\ T = \left(T_1 \vec{\cup} T_2\right) \cup \left(T_1 \cup \downarrow T_2\right), T_1 \cap T_2 \neq \varnothing. \end{cases}$	(2.9)	10	Taxonomic combining and attributive combining of hierarchical structures without intersection of taxons sets (Fig. 11m) $\begin{cases} A = A_1 \cup A_2, A_1 \cap A_2 \neq \varnothing; \\ T = \left(T_1 \vec{\cup} T_2\right) \cup \left(T_1 \cup \downarrow T_2\right), T_1 \cap T_2 = \varnothing. \end{cases}$	(2.10)

Table 4 Formal description of facet structures combined variants

1	Taxonomic combining of facet structures without intersection of taxons sets (Fig. 12a) $\begin{cases} F = F_1; \\ T = T_1 \vec{\cup} T_2, T_1 \cap T_2 = \varnothing. \end{cases}$	(2.11)	2	Taxonomic combining of facet structures with intersection of taxons sets (Fig. 12b) $\begin{cases} F = F_1; \\ T = T_1 \vec{\cup} T_2, T_1 \cap T_2 \neq \varnothing. \end{cases}$	(2.12)
3	Attributive combining of facet structures without intersection of taxons sets and with intersection of classification attributes (Fig. 12c) $\begin{cases} F = F_1 \cup F_2, F_1 \cap F_2 \neq \varnothing; \\ T = T_1 \cup \downarrow T_2, T_1 \cap T_2 = \varnothing. \end{cases}$	(2.13)	4	Attributive combining of facet structures without intersection of taxons sets and without intersection of classification attributes (Fig. 12d) $\begin{cases} F = F_1 \cup F_2, F_1 \cap F_2 = \varnothing; \\ T = T_1 \cup \downarrow T_2, T_1 \cap T_2 = \varnothing. \end{cases}$	(2.14)
5	Attributive combining of facet structures with intersection of taxons sets (Fig. 12e) $\begin{cases} F = F_1 \cup F_2, F_1 \cap F_2 \neq \varnothing; \\ T = T_1 \cup \downarrow T_2, T_1 \cap T_2 \neq \varnothing. \end{cases}$	(2.15)	6	Combining of facet structures with inclusion of taxons sets (Fig. 12f) $\begin{cases} F = F_1; \\ T = T_1. \end{cases}$	(2.16)
7	Combining of facet structures with equality of taxons sets (Fig. 12j) $\begin{cases} F = F_1 = F_3; \\ T = T_1 = T_3. \end{cases}$	(2.17)	8	Combining of facet structures in facet-hierarchical structure (Fig. 12k) $\begin{cases} F = F_1 \cup_{FHS} F_2, F_1 \cap F_2 = \varnothing; \\ T = T_1 \cup_{FHS} T_2, T_1 \cap T_2 = \varnothing. \end{cases}$	(2.18)
9	Taxonomic combining and attributive combining of facet structures with intersection of taxons sets (Fig. 12l) $\begin{cases} F = F_1 \cup F_2, F_1 \cap F_2 \neq \varnothing; \\ T = \left(T_1 \vec{\cup} T_2\right) \cup (T_1 \cup \downarrow T_2), T_1 \cap T_2 \neq \varnothing. \end{cases}$	(2.19)	10	Taxonomic combining and attributive combining of facet structures without intersection of taxons sets (Fig. 12m) $\begin{cases} F = F_1 \cup F_2, F_1 \cap F_2 \neq \varnothing; \\ T = \left(T_1 \vec{\cup} T_2\right) \cup (T_1 \cup \downarrow T_2), T_1 \cap T_2 = \varnothing. \end{cases}$	(2.20)

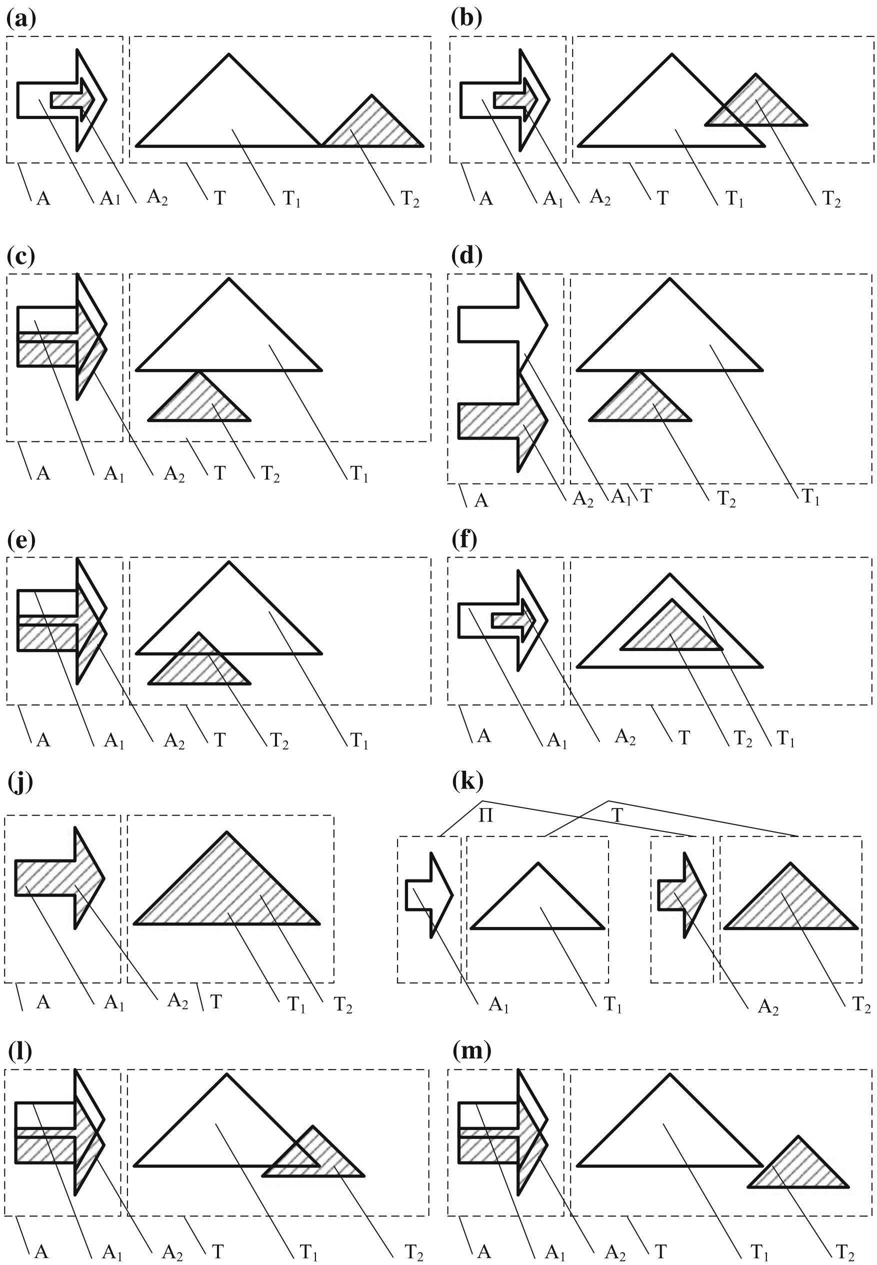


Fig. 11 Graphic representation of hierarchical structures variants combining

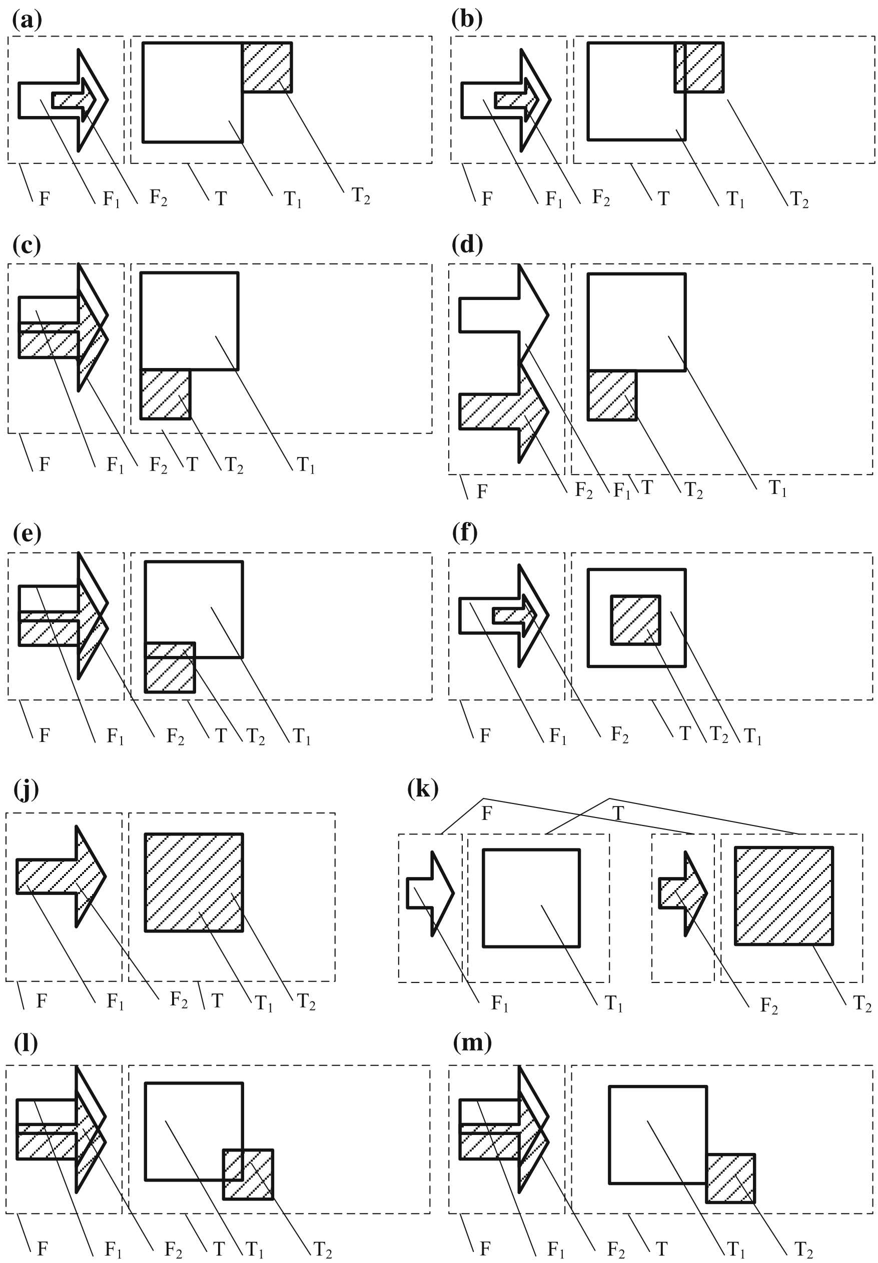


Fig. 12 Graphical representation of variants of facet structures combining

3.5 Operation of Decomposition

Operation of decomposition of taxonomic structures consists of decomposition of sets A and T into subsets. Some terms, which are needed for description of taxonomic structures decomposition operation have been introduced: Tres—a set of taxons of residual taxonomic structure; Tres.i—initial set of taxons of residual taxonomic structure; Tres.red—reduced set of taxons of residual taxonomic structure; Tdes—a set of taxons of desired taxonomic structure; Tdes.i—initial set of taxons of desired taxonomic structure; Tdes.red—reduced set of taxons of desired taxonomic structure; Tstrt—a set of taxons of starting taxonomic structure; initial taxonomic structure—structure before execution over its operation of decomposition; desired taxonomic structure—structure after execution of operation of decomposition; residual taxonomic structure—addition of structure to of initial taxonomic structure.

Following types of hierarchical structures decomposition (attributive and taxonomic decomposition) have considered. Attributive decomposition of hierarchical structures consists in choice of hierarchical structure, proceeding from semantic compliance between elements of sets A and C (set of choice criteria). Attributive decomposition cannot be used to hierarchical structures, because set A in hierarchical structures is indivisible and fixed.

Taxonomic decomposition of hierarchical structures consists of forming of set $T_{des} \subset T$ for hierarchical structures. Set T_{des} is determined on the basis of semantic compliance between elements of sets T and C. Semantic equivalents are determined by expert. We represent taxonomic decomposition by the following stages.

Stage 1. Forming of initial data: hierarchical structure by represented of contiguity matrix, compliance matrix of elements of sets T and A, set C.

Stage 2. Establishment of equivalence between elements of taxons set and choice criteria. Initial data is given in sets of T and C. Semantic equivalents between elements of sets T and C are determined by expert.

Stage 3. Receive of sets T_{des} and T_{res}. For this:

- set $T_{des.i}$ has been defined. Elements of set is elements of set T_{des}, with which was established compliance of elements of set C. $T_{des.i} = \{t_i, t_{i+1}, \ldots, t_n\}$;
- set $T_{des.red}$ has been defined;
- set $T_{des.}$ as a result of combining $T_{des.i}$ and $T_{des.red}$ has been defined:

$$T_{des} = T_{des.i} \cup T_{des.red}, T_{des.i} \cap T_{des.red} \neq \varnothing;$$

- set T_{res} set $T_{des.red}$ has defined. For this we define $T_{des.i.}$. This is a set is symmetric difference of T_{strt} and T_{des}, $T_{res.i} = T_{strt} \backslash T_{des}$;
- set $T_{res.red}$ set $T_{des.red}$ have been defined;
- set T_{res} on basis combining $T_{res.i}$ and $T_{res.red}$ have been formed:

$$T_{res} = T_{res.i} \cup T_{res.red}, T_{res.i} \cap T_{res.red} \neq \varnothing.$$

Stage 4. Correction of completeness set T_{des} for classification attributes. This is stage typical only for attributive decomposition of facet structures. Expert can precise of set T_{des} for classification attributes.

The following types of decomposition facet structures: attributive decomposition and taxonomic decomposition have been considered.

Attributive decomposition of facet structures consists of choice of facet structure, proceeding from semantic compliance of elements of sets A and C.

This type of decomposition included in all stages, which description in operation of taxonomic decomposition of hierarchical structure is:

- on the second stage determined semantic compliance between elements of sets A and C;
- on the fourth stage produced correction of completeness sets T_{des} for classification attributes.

Taxonomic decomposition of hierarchical structures consists of choice of facet structure, i.e. set T_{des}, proceeding from semantic compliance of elements sets T и C.

This type of decomposition included all stages, which description in the operation of taxonomic decomposition of hierarchical structures, excluding stage №4.

3.6 Semantic Issues

In this work the operation of combining and decomposition is considered in the context of structures (taxonomic) excluding their semantic context. The analysis of semantic context of taxonomic structures with operations of combining and decomposition will give the following opportunities:

- firstly, consider taxonomic structures not only on structural level, but and on semantic level of individual nodes;
- secondly, take into account features of semantic structures for their formal description (representation);
- in the third, determine limitations at use of operations of combining and decomposition on structural level and semantic level.

3.7 Profiling Sequence

Basic stages of profiling have considered.

Stage 1. Transformation initial information in FHS. The goal of this stage is transformation of information in facet hierarchical structure. Dedication such operations in separate stage connected with absence of formalization in initial information about requirements. Such work demand of considerable time expense.

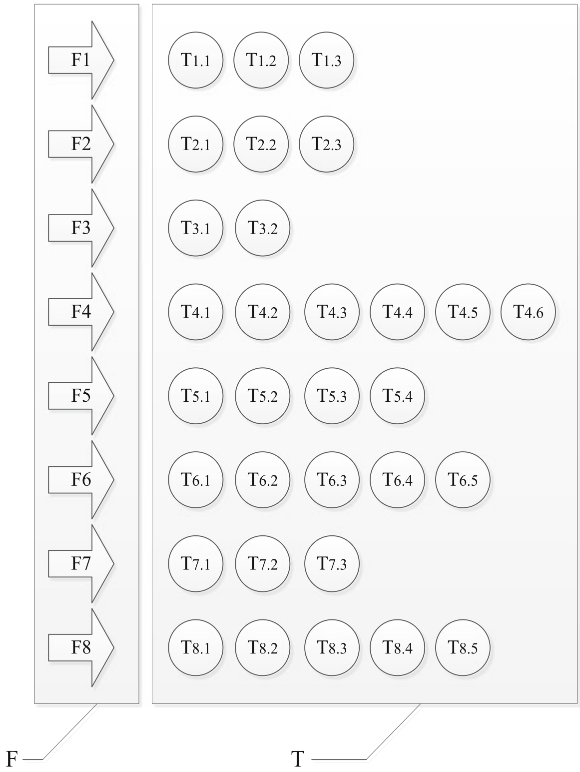


Fig. 13 Facet structure for ISO/IEC 25010

Stage 2. Representation of FHS in set-matrix look. The basic task of this stage is representation of FHS in look of matrices (contiguity matrix and compliance matrix for hierarchical structures, compliance matrix for facet structures) and establish of variant of combining or decomposition of FHS.

Stage 3. Choice of operation type. The basic task of this stage is determination of operation (combining and decomposition) for forming of software requirements profile.

Stage 4. Choice of profile. Stage needed, when FHS use iteratively. Basic task this opportunity of download of FHS from database.

Stage 5. Operation of combining (or decomposition) of facet and hierarchical structures. Stage needed for realization of combining (or decomposition) of FHS in according with their types and establishing of combining type (or decomposition).

Stage 6. Forming and description of requirements profile. Requirements profile on the basis of selected operation of taxonomic structure transformation has been received. Further created profile must be description for repeated his use.

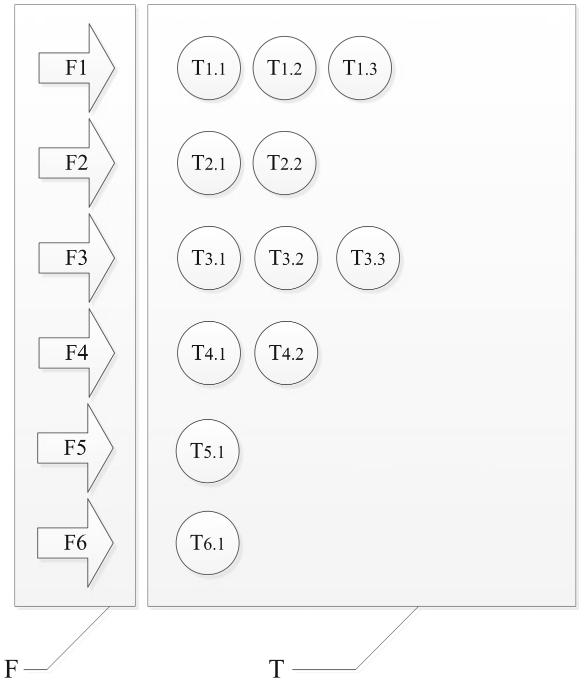


Fig. 14 Facet structure for GAMP

4 Case Study: Profiling of Requirements to PE MES Software

4.1 Profiling Procedure

Let us receive the generalized software requirements MES profile. The software requirements profile will have developed for initial data. In this case software MES requirements profile based on [12] and GAMP (Good Automated Manufacturing Practice) for software validation [13]. Let's represent short characteristic of these standards:

1. ISO/IEC 25010 standard "Systems and software—Systems and software Quality Requirements and Evaluation (SQuaRE)—System and software quality models" standard defines: (a) A quality in use model composed of five characteristics (some of which are further subdivided into subcharacteristics) that relate to the outcome of interaction when a product is used in a particular context of use. This system model is applicable to the complete human-computer system, including both computer systems in use and software products in use; (b) A product quality model composed of eight characteristics (which are further subdivided into sub-characteristics) that relate to static properties of software and dynamic properties

Table 5 Compliance matrix of facet structure

	F_1	F_2	F_3	F_4	F_5	F_6	F_7	F_8
$T_{1.1}$	1	0	0	0	0	0	0	0
$T_{1.2}$	1	0	0	0	0	0	0	0
$T_{1.3}$	1	0	0	0	0	0	0	0
$T_{2.1}$	0	1	0	0	0	0	0	0
$T_{2.2}$	0	1	0	0	0	0	0	0
$T_{2.3}$	0	1	0	0	0	0	0	0
$T_{3.1}$	0	0	1	0	0	0	0	0
$T_{3.2}$	0	0	1	0	0	0	0	0
$T_{4.1}$	0	0	0	1	0	0	0	0
$T_{4.2}$	0	0	0	1	0	0	0	0
$T_{4.3}$	0	0	0	1	0	0	0	0
$T_{4.4}$	0	0	0	1	0	0	0	0
$T_{4.5}$	0	0	0	1	0	0	0	0
$T_{4.6}$	0	0	0	1	0	0	0	0
$T_{5.1}$	0	0	0	0	1	0	0	0
$T_{5.2}$	0	0	0	0	1	0	0	0
$T_{5.3}$	0	0	0	0	1	0	0	0
$T_{5.4}$	0	0	0	0	1	0	0	0
$T_{6.1}$	0	0	0	0	0	1	0	0
$T_{6.2}$	0	0	0	0	0	1	0	0
$T_{6.3}$	0	0	0	0	0	1	0	0
$T_{6.4}$	0	0	0	0	0	1	0	0
$T_{6.5}$	0	0	0	0	0	1	0	0
$T_{7.1}$	0	0	0	0	0	0	1	0
$T_{7.2}$	0	0	0	0	0	0	1	0
$T_{7.3}$	0	0	0	0	0	0	1	0
$T_{8.1}$	0	0	0	0	0	0	0	1
$T_{8.2}$	0	0	0	0	0	0	0	1
$T_{8.3}$	0	0	0	0	0	0	0	1
$T_{8.4}$	0	0	0	0	0	0	0	1
$T_{8.5}$	0	0	0	0	0	0	0	1

of the computer system. The model is applicable to both computer systems and software products.

2. "Good Automated Manufacturing Practice" (GAMP) [13] is a standard for validation of automated systems for pharmaceutical branch. This standard regulates the main phases of systems development life cycle for PE software. According to GAMP software suppliers and software users must be responsible and carefully abide validation procedures.

Table 6 Compliance of taxons indexes with taxon names

$T_{1.1}$	Functional completeness
$T_{1.2}$	Functional correctness
$T_{1.3}$	Functional appropriateness
$T_{2.1}$	Time-behavior
$T_{2.2}$	Resource utilization
$T_{2.3}$	Capacity
$T_{3.1}$	Co-existence
$T_{3.2}$	Interoperability
$T_{4.1}$	Appropriateness recognisability
$T_{4.2}$	Learnability
$T_{4.3}$	Operability
$T_{4.4}$	User error protection
$T_{4.5}$	User interface aesthetics
$T_{4.6}$	Accessibility
$T_{5.1}$	Maturity
$T_{5.2}$	Availability
$T_{5.3}$	Fault tolerance
$T_{5.4}$	Recoverability
$T_{6.1}$	Confidentiality
$T_{6.2}$	Integrity
$T_{6.3}$	Non-repudiation
$T_{6.4}$	Accountability
$T_{6.5}$	Authenticity
$T_{7.1}$	Adaptability
$T_{7.2}$	Installability
$T_{7.3}$	Replaceability
$T_{8.1}$	Modifiability
$T_{8.2}$	Testability
$T_{8.3}$	Modularity
$T_{8.4}$	Reusability
$T_{8.5}$	Analyzability

4.2 Initialization Data

According to profiling algorithm stages has defined taxonomic structure types and conceptual represented the initial profiles. In this case initial profile represents with facet structures (Figs. 13 [12] and 14 [13]).

Initial facet structures have described in set-matrix view.

Facet structure (Fig. 13) of PE MES requirements profile [12], consists of sets $F = \{F_1, F_2, F_3, F_4, F_5, F_6, F_7, F_8\}$ and $T = \{T_{1.1}, T_{1.2}, T_{1.3}, T_{2.1}, T_{2.2}, T_{2.3}, T_{3.1},$ $T_{3.2}, T_{4.1}, T_{4.2}, T_{4.3}, T_{4.4}, T_{4.5}, T_{4.6}, T_{5.1}, T_{5.2}, T_{5.3}, T_{5.4}, T_{6.1}, T_{6.2}, T_{6.3}, T_{6.4}, T_{6.5},$

Table 7 Compliance of classification attributes (facets) indexes with facets names

	Classification attributes name
F_1	Functional Suitability
F_2	Performance efficiency
F_3	Compatibility
F_4	Usability
F_5	Reliability
F_6	Security
F_7	Portability
F_8	Maintainability

Table 8 Compliance matrix of facet structure

	F_1	F_2	F_3	F_4	F_5	F_6
$T_{1.1}$	1	0	0	0	0	0
$T_{1.2}$	1	0	0	0	0	0
$T_{1.3}$	1	0	0	0	0	0
$T_{2.1}$	0	1	0	0	0	0
$T_{2.2}$	0	1	0	0	0	0
$T_{3.1}$	0	0	1	0	0	0
$T_{3.2}$	0	0	1	0	0	0
$T_{3.3}$	0	0	1	0	0	0
$T_{4.1}$	0	0	0	1	0	0
$T_{4.2}$	0	0	0	1	0	0
$T_{5.1}$	0	0	0	0	1	0
$T_{6.1}$	0	0	0	0	0	1

Table 9 Compliance of taxons indexes with taxons name

	Taxon Names
$T_{1.1}$	Functional correctness
$T_{1.2}$	Response
$T_{1.3}$	Synchronization
$T_{2.1}$	Bandwidth
$T_{2.2}$	Access speed
$T_{3.1}$	User interface
$T_{3.2}$	Interface with another systems
$T_{3.3}$	Interface with another equipments
$T_{4.1}$	Physical allocation
$T_{4.2}$	Physical conditions
$T_{5.1}$	Reliability
$T_{6.1}$	Security

$T_{7.1}$, $T_{7.2}$, $T_{7.3}$, $T_{8.1}$, $T_{8.2}$, $T_{8.3}$, $T_{8.4}$, $T_{8.5}$} in the form of compliance matrix has represented (Table 5). For better understanding of profiling procedure taxons name (Table 6) and classification attributes (facets) of initial taxonomic (facet) structures have represented in Table 7.

Table 10 Compliance of classification attributes (facets) indexes with facets names

	Classification attributes name
F_1	Functional
F_2	Data
F_3	Interfaces
F_4	Environment
F_5	Reliability
F_6	Security

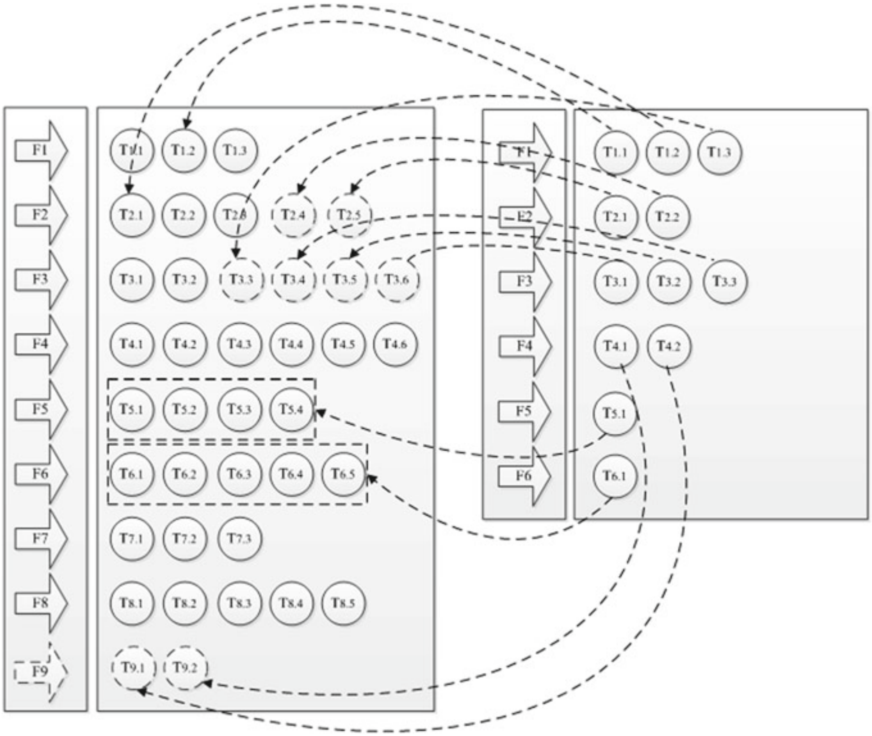


Fig. 15 Result of software requirements profiles profiling

Facet structure (Fig. 14) of requirements profile [13] consists of sets F = {F_1, F_2, F_3, F_4, F_5, F_6} and T = {$T_{1.1}$, $T_{1.2}$, $T_{1.3}$, $T_{2.1}$, $T_{2.2}$, $T_{3.1}$, $T_{3.2}$, $T_{3.3}$, $T_{4.1}$, $T_{4.2}$, $T_{5.1}$, $T_{6.1}$} in the form of compliance matrix has represented (Table 8). For better understanding of profiling procedure taxons name (Table 9) and classification attributes (facets) of initial taxonomic (facet) structures have represented in Table 10.

4.3 Profiling Results

Initial software requirements profiles have represented in the form of facet structures. In this connection for forming of generalized software requirements profile has used of operation of combining facet structures. As a result of operation combining software requirements profiles, which represented in the form of initial facet structures have received generalized software requirements profile (Fig. 15).

5 Conclusions

In this chapter international standards, which describes the PE MES requirements software have considered.

SFHS-based technique for formal description and formation of profiles requirements has proposed. Within the framework of SFHS-based technique set of terms and connection between them have represented (Fig. 6). Possible variants of combining hierarchical (Fig. 11) and facet structures (Fig. 12) have reviewed. SFHS-based technique can be applied to develop profiles requirements to PE MES taking into account their features. To illustrate the approach and technique example of generalized forming process profile to the PE MES requirements was analyzed.

Future work will be connected with the development of tools to support the requirements profiling process and case-based assessment of PE software quality and safety.

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