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MATHEMATICS METHODS AND INFORMATION SYSTEMS IN CHEMICAL TECHNOLOGY
МАТЕМАТИЧЕСКИЕ МЕТОДЫ И ИНФОРМАЦИОННЫЕ СИСТЕМЫ В ХИМИЧЕСКОЙ ТЕХНОЛОГИИ

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Verification of functional models of chemical manufacturing

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A generalized algorithm for the verification of functional models and the rules for the verification of diagrams related by levels of detail were developed in this paper. The algorithm is based on the analysis of a tree which describes the decompose relations in functional diagrams. At each step of the algorithm, a pair consisting of a parent diagram and a functional diagram is selected, and the correlation of the arrows and their roles is checked for both. The formalization of the verification rules was based on the set-theoretic representation of functional diagrams in the form of labeled oriented graphs. The rules make it possible to map the position and roles of the arrows associated with the detailed function block of the parent diagram to the arrows of the child diagram. The following rules for each of the possible arrow roles were established: "input", "output", "control", "mechanism". The use of the logic programming language PROLOG was proposed for the implementation of the algorithm. A knowledge base structure comprised of 3 interrelated predicates to describe the tree of diagrams, nodes and edges of the graphs was suggested. A query to check the verification rules was formed, and methods of binding variables and fixing roles were considered. The analysis and verification of a fragment of a functional model for the production of vinyl acetate from ethylene was conducted as an example. The functional diagrams for the processes "Condensate separation" and "Vinyl acetate isolation" connected by a decompose relation were developed, their set-theoretic models were constructed, and the use of rules for the verification of each type of arrow were considered.

Keywords: *functional modeling, functional model verification, set theory, graph theory, vinyl acetate production.*

Верификация функциональных моделей химических производств

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Разработан обобщенный алгоритм верификации функциональных моделей и правила проверки связанных отношением детализации диаграмм. Алгоритм основан на анализе дерева, описывающего отношение детализации функциональных диаграмм. На каждом шаге алго-

ритма выбирается пара, состоящая из родительской и функциональной диаграмм, и для этой пары выполняется проверка соответствия стрелок и их ролей. Формализация правил проверки выполнена на основе теоретико-множественного представления функциональных диаграмм в виде помеченных ориентированных графов. Правила позволяют сопоставить положение и роли стрелок, связанных с детализируемым функциональным блоком родительской диаграммы, и стрелок дочерней диаграммы. Построены правила для каждой из возможных ролей стрелки: «вход», «выход», «управление», «механизм». Для реализации построенного алгоритм предложено использование языка логического программирования ПРОЛОГ. Предложена структура базы знаний, включающая 3 взаимосвязанных предиката для описания дерева детализации, вершин и дуг графов, задающих функциональные диаграммы. Сформирован запрос для проверки правил верификации, рассмотрены способы связывания переменных и фиксации ролей. В качестве примера выполнен анализ и верификация фрагмента функциональной модели получения винилацетата из этилена. Приведены функциональные диаграммы для процессов «Разделение конденсата» и «Получение винилацетата», связанных отношением детализации, построены их теоретико-множественные модели, рассмотрено применение правил верификации для каждого типа стрелок.

Ключевые слова: *функциональное моделирование, верификация функциональной модели, теория множеств, теория графов, получение винилацетата.*

Introduction

Enhancing the efficiency of the Russian chemical industry with continuous modernization and the manufacturing improvement is one of the most important and pressing objectives. The methodology of functional modeling is intended for the design, description and analysis of manufacturing systems in order to increase their efficiency [1, 2].

As a rule, the main advantages of functional modeling methodology when compared to other means of describing production and organizational processes are considered to be its convenience for specialists of various profiles, as well as the freedom from restrictions on the level of detail [3–5]. The possibility of a strict formalization of functional models, their analysis and verification are discussed in specialized literature [6, 7] and has been implemented in a set of commercial software products designed to create functional models[1,2] [8]. However, the objective of developing rules and algorithms for checking functional models has not yet been achieved.

Generalized algorithm for functional model verification

According to [9], a functional model is a set of diagrams connected by a decompose relation. The model structure can be represented as a tree. Each branch of this tree presets a pair comprised of a parent and child diagram, the latter detailing one of the parent diagram's functional blocks.

[1]Internet source: https://www.ca.com/us.html

[2]Internet source: https://www.edrawsoft.com/IDEF0-flowcharts.php

Each arrow associated with the detailed functional block must have a corresponding boundary arrow in the child diagram. Its role is uniquely determined by the role of the corresponding arrow in the parent diagram. In order to check the correctness of the functional model, all the relationships between the parent and child diagrams must be analyzed, and the presence and roles of arrows must be confirmed. A generalized algorithm for functional model verification is shown in Fig. 1.

This algorithm demonstrates a sequential search for diagrams connected by a decompose relation, the choice of arrows that must be displayed in child diagrams and the verification of their roles. (This verification will be discussed below in more detail).

In order to formalize this algorithm, it is necessary to switch from the visual representation of functional models in the form of graphical diagrams to their mathematical descriptions.

The formalization of rules for the verification of functional models based on their set-theoretic representations

In [10] a set-theoretic representation of functional models as a set of special oriented graphs related by levels of detail is proposed in this study. Such a representation allows for the possibility of using the mathematical apparatus accumulated within the framework of graph theory [11] for verifying and analyzing functional diagrams.

A separate functional diagram is not a graph as a diagram can contain boundary and branching arrows, while the edges of a graph connect precisely two of its nodes. It is essential that the semantics of the actions described by a functional diagram is preset not only by

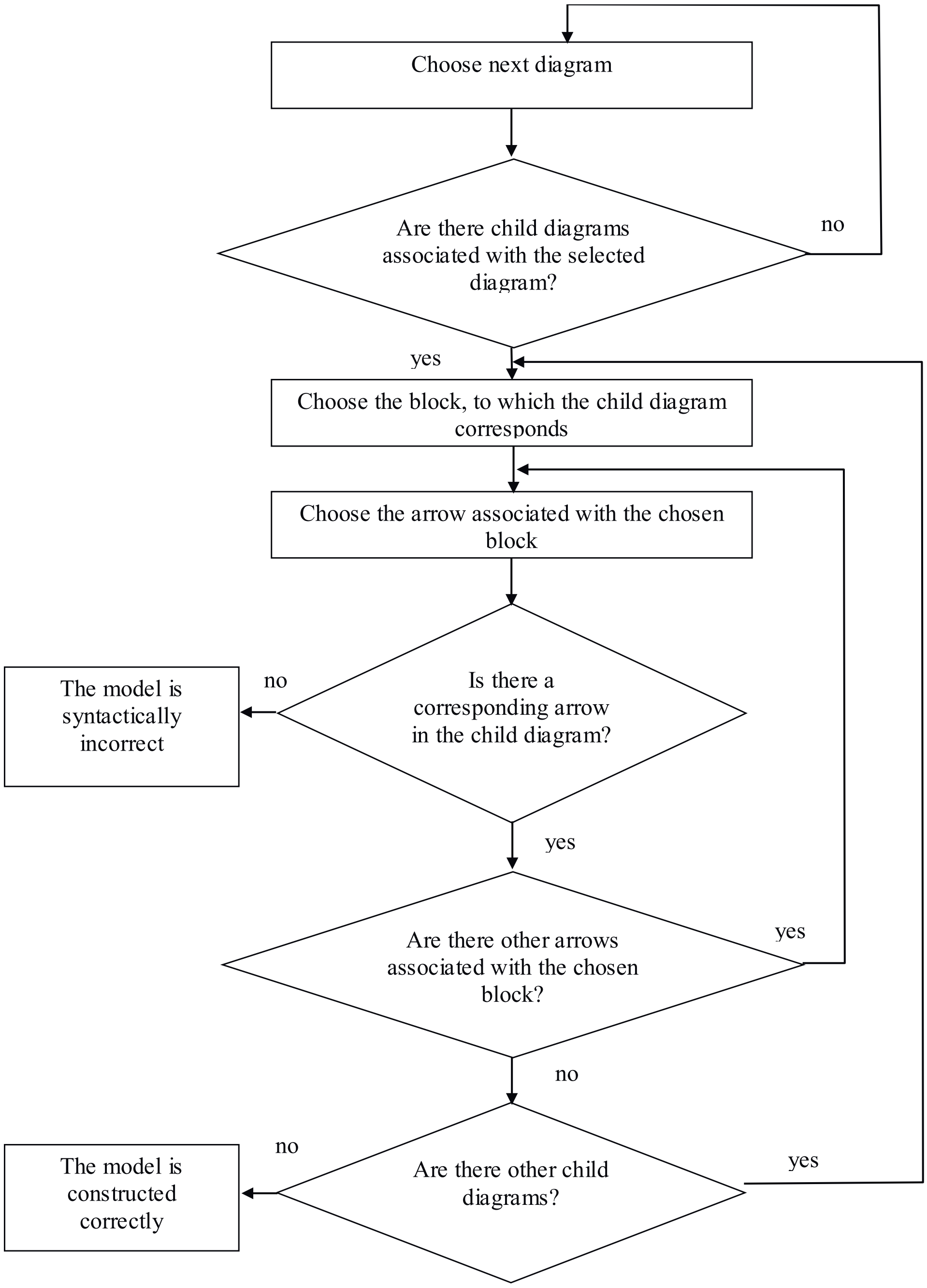

Fig. 1. Algorithm for functional model verification.

the edge name, but also by its position relative to the functional block. A detailed description of a diagram conversion into a graph is given in [10]. Below is a brief list of its main features:

- The diagram is represented as a graph with labeled edges G = (N, L), where N is the set of nodes and L is the set of edges.
- The graph nodes preset functional blocks, diagram boundaries, and the branch points of the arrows.
- Each edge of the graph has a label, which is not necessarily unique.
- When specifying the edges of a graph, both the names of the nodes and their roles must be indicated. Each edge of the graph is described as follows:

**edge name (initial_node_role:
initial_node_Name,
end_node_role:
end_node_Name)**

In order to formalize the rules of model verification we introduce the following notations:

DP = (NP, LP) is a graph describing the parent diagram;

NP is the set of the DP graph nodes;

LP is the set of the DP graph edges;

(DP, DC, nb) is an element of the decompose relation that describes the decomposition of the nb block of the parent diagram, nb $\in$ NP;

DC = (NC, LC) is a graph describing the child diagram;

NC is the set of the DC graph nodes;

LC is the set of the DC graph edges;

$np \in NP$ is an element of the NP set, $np \neq nb$;

$nc \in NC$ is an element of the NC set.

Let us consider the rules, which connect the elements of the LP and LC sets (the edges of graphs describing the parent and child diagrams):

1) Each arrow of the parent diagram, which points to the nb block on the left, has at least one corresponding arrow in the child diagram. The latter arrow has the same label; it goes from the left border of the diagram and points to a block of the child diagram on the left:

if lp(O:np, I:nb) ∈ LP, then lp(O:L, I:nc) ∈ LC

2) Each arrow of the parent diagram, which emerges from the nb block, has at least one corresponding arrow in the child diagram. The latter arrow has the same label; it points to the right border of the diagram from a block of the child diagram:

if lp(O:nb, I:np) ∈ LP, then lp(O:nc, I:R) ∈ LC

3) Each arrow of the parent diagram, which points to the nb block above, has at least one corresponding arrow in the child diagram. The latter arrow has the same label; it goes from the top border of the diagram and points to a block of the child diagram above:

if lp(O:np, C:nb) ∈ LP, then lp(O:U, C:nc) ∈ LC

4) Each arrow of the parent diagram, which points to the nb block below, has at least one corresponding arrow in the child diagram. The latter arrow has the same label; it goes from the bottom border of the diagram and points to some block of the child diagram below:

if lp(O:np, M:nb) ∈ LP, then lp(O:D, M:nc) ∈ LC

The np and nc nodes can describe both blocks of the corresponding functional diagrams and their boundaries or branch points. Note also that one arrow of the parent diagram may correspond to several arrows of the child diagram in cases when the arrow in the child diagram branches without changing its label.

Programming languages, which contain convenient means for describing and analyzing relationships, as well as pattern matching tools, are suitable for the implementation of the functional model verification algorithm. The most convenient logic programming language for this task is PROLOG, which supports predicate notation for storing relations and provides sophisticated means for describing logical rules with related variables [12]. A knowledge base is necessary in order to store a functional model in the PROLOG language. It includes 3 predicates: descriptions of the decompose relation (decompose), of the nodes set (node), and of the edges set (edge). The rules for model verification are a conjunction of these predicates, and constraints are described using role specifying and variable binding. Thus, the first rule describing the correlation between arrows with the "input" role can be verified using the following query:

```
?-decompose(DP,DC,NB),
  edge(LP,o,NP,i,NB),
  edge(LP,o,l,i,NC),
  node(NC,DC).
```

In this query, according to PROLOG rules, the capitalized variables signify:

DP is the parent diagram name;

DC is the child diagram name;

NB is the name of the detailed function block;

LP is the label of the parent diagram edge;

NP is the name of the initial node of the LP edge in the parent diagram;

NC is the name of the final node of the LP edge in the child diagram.

The lowercase letters o and i define the roles of the nodes. The lowercase letter l describes the node corresponding to the diagram left border.

An example of verifying the fragment of a functional model of vinyl acetate production from ethylene

Let us consider the verification of diagram construction using a functional model for vinyl acetate production from ethylene as an example. A generalized technological scheme of this production was given in [13], and its functional and set-theoretic models were built in [10]. For example, let us chose the level A4 "Condensate separation" diagram as a parent diagram (Fig. 2).

The figure shows that this diagram consists of 4 functional blocks. Each of them is decomposed into a separate child diagram. Let us consider the relationship of the "Condensate separation" diagram and the "Vinyl acetate isolation" diagram. The latter describes the preparation of the target product – vinyl acetate. This diagram level is A44, and it represents the result of the decomposition of the last, fourth functional block of the

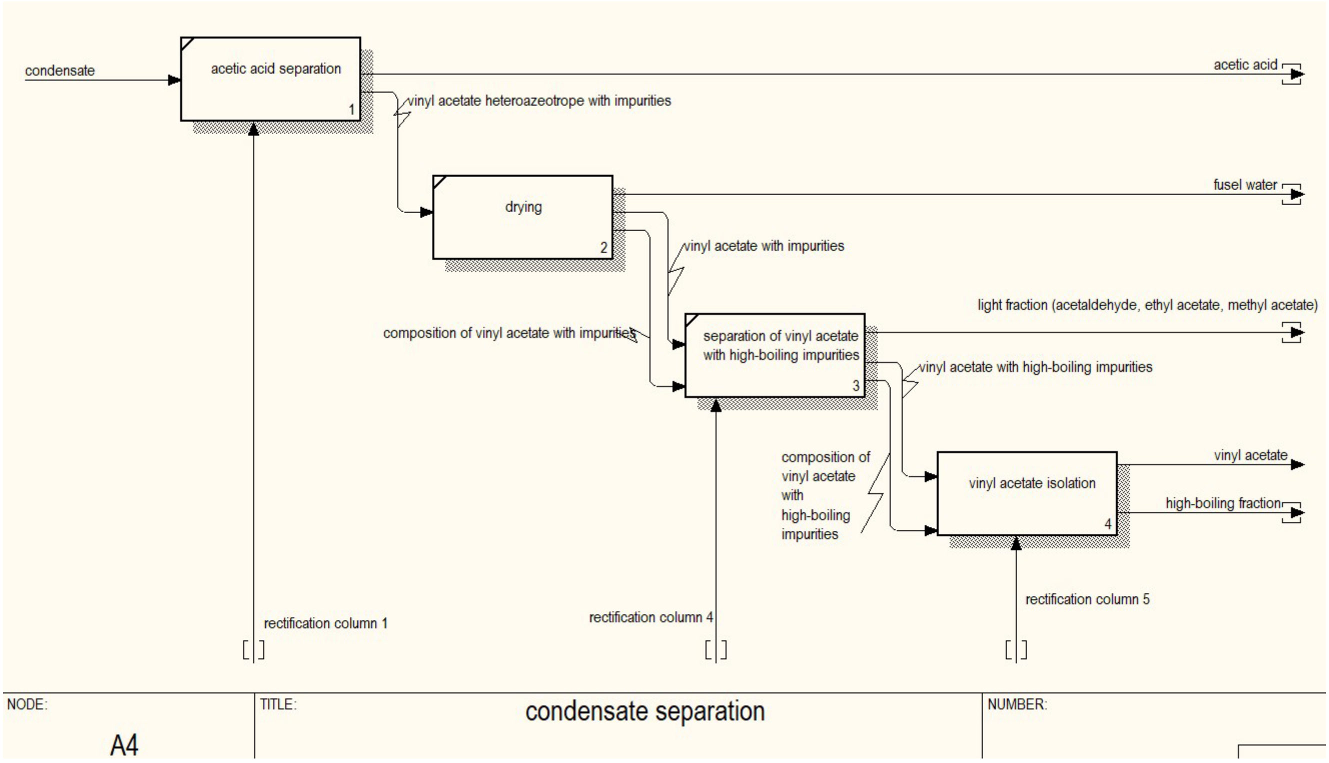

Fig. 2. Parent functional diagram "Condensate separation".

A4 = (N4; L4), where

N4 = {L, R, U, D, Acetic_acid_separation, Drying, Separation_of_vinyl_acetate_with_high-boiling_impurities, ***Vinyl_acetate isolation***}

L4 ⊃ {composition_of_vinyl_acetate_with_high-boiling_impurities
(O:Separation_of_vinyl_acetate_with_high-boiling_impurities,
I: ***Vinyl_acetate_isolation***)

vinyl_acetate_with_high-boiling_impurities
(O: Separation_of_vinyl_acetate_with_high-boiling_impurities,
I: ***Vinyl_acetate_isolation***)

rectification_column_5(*O: D, M:* ***Vinyl_acetate_isolation***)

vinyl_acetate(O: ***Vinyl_acetate_isolation***, I: R)

high-boiling_fraction(O: ***Vinyl_acetate_isolation***, I: R)}

Fig. 3. A set-theoretic representation of the functional diagram "Condensate separation" (fragment).

parent diagram. Thus, we are analyzing an element of the decompose relation

(A4, A44, Vinyl acetate isolation).

Fig. 2 demonstrates that two arrows with the "input" role and one arrow with the "mechanism" role enter the "Vinyl acetate isolation" functional block in the "Condensate separation" diagram. Two arrows with the "exit" role go out of this block. Let us consider a fragment of the set-theoretic description of the parent diagram (Fig. 3). Graph A4 consists of a set of nodes N4 (this set is shown in Fig. 3 completely) and a set of edges L4 (a subset of this set is shown, including edges associated with the "Vinyl acetate isolation" node). For clarity, the edge labels are in italics, and the decomposed node name is in bold italics.

The diagram obtained as a result of the "Vinyl acetate isolation" functional block decomposition is shown in Fig. 4. Let us analyze graph A44 that defines its set-theoretic representation (Fig. 5).

The set of nodes of this graph (N44) includes only 2 nodes corresponding to the diagram functional blocks and 4 service nodes. Since the name of one of the

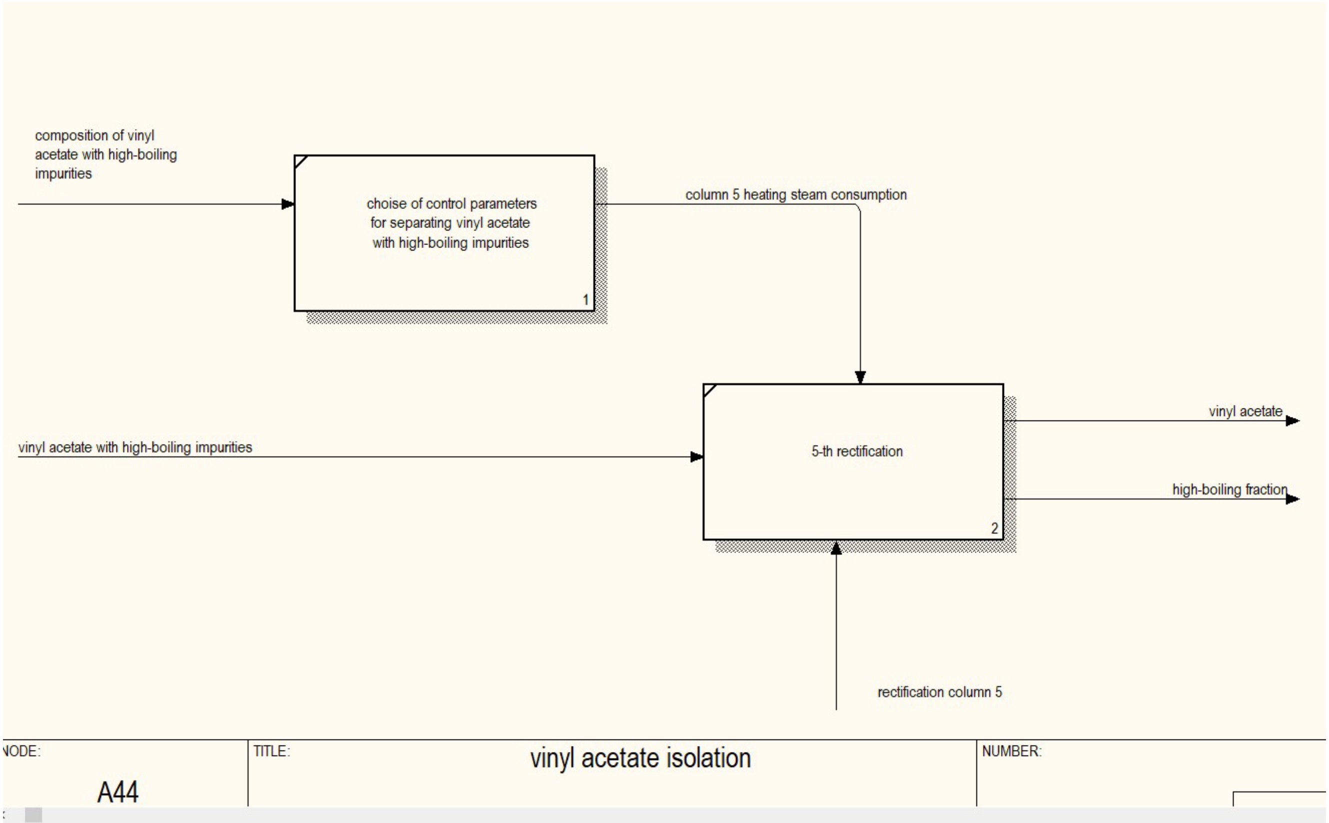

Fig. 4. Child functional diagram
"Vinyl acetate isolation"

A44={N44;L44}, where
N44 = {L, R, U, D, Choice_of_control_parameters, 5th_rectification}
L44 = {*composition_of_vinyl_acetate_with_high-boiling_impurities*
(O:L, I: Choice_of_control_parameters)
vinyl_acetate_with_high-boiling_impurities(O:L, I: 5th_rectification)
rectification_column_5(O:D,M: 5th_rectification)
high-boiling fraction(O: 5th_rectification,I:R)
vinyl_acetate(O: 5th_rectification,I:R)
column_5_heating_steam_consumption
(O: Choice_control_parameters, I: 5th_rectification)}

Fig. 5. A set-theoretic representation of the functional diagram
"Vinyl acetate isolation".

blocks is very long, the name of the node describing it is abbreviated. The set of edges in graph L44 is shown in Fig. 5 completely; as before, the edge labels are in italics.

Let us compare the descriptions of the edges of the parent and child diagrams. In the parent diagram, the "vinyl_acetate_with_high-_boiling_impurities" arrow leads from block 3 to block 4. For the "vinyl acetate isolation" block, this arrow has the "input" role. In the child diagram, this arrow corresponds to the arrow leading from the left border of the diagram to the "Choice_control_parameters" block.

The set-theoretic description of these arrows should correspond to rule 1, where

nb = "Vinyl acetate isolation",

lp = "Vinyl_acetate_with_high-_boiling_impurities",

nc = "Choice_control_parameters".

The verification shows that the rule is obeyed.

Similarly, in the parent diagram, an arrow with the role "mechanism" leads from the bottom border of the diagram to the "Vinyl acetate isolation" block. In the child diagram, this arrow corresponds to an arrow that also leads from the bottom border to the "5th rectification" function block. The set-theoretic description of these arrows should correspond to rule 4, where

nb = "Vinyl acetate isolation",

lp = "Rectification_column_5",

nc = "5th rectification"

The analysis of the remaining arrows of the parent and child diagrams shows that each edge of the parent diagram corresponds to one edge of the child diagram. The latter corresponds to either rule 1, or rule 2, or rule 4. The child diagram has a single arrow unassociated with the parent diagram: the arrow "column_5_heating_steam_consumption".

Thus, it has been shown that the decomposition of the function block "Vinyl acetate isolation" has been performed correctly.

Conclusion

The algorithm for functional model verification is based on analyzing a tree which describes the level of detail of functional diagrams. At each step of the algorithm, a pair consisting of a parent and child diagrams is selected, and the rules for arrow correlation in these diagrams are checked. To formalize these rules, a set-theoretic representation of the diagrams in the form of graphs is utilized. The rules are implemented with the use of the PROLOG logic programming language.

The authors declare no conflict of interest.

References:

1. Cheremnyh S.V., Semenov I.O., Ruchkin V.S. Modelling and system analysis. IDEF technology. Moscow: Finansy i statistika Publ., 2006. 192 p. (in Russ.).

2. Myshenkov K.S. Justification technique of a choice of CASE-tools for the analysis and design of management systems by enterprise. *Innovatsii* [Innovations]. 2013;10(180):112-122 (in Russ.).

3. Erusheva K., Kolybanov K., Tishaeva I. Functional modeling of the process of choosing the best available technique. *Tonkie Khimicheskie Tekhnologii = Fine Chemical Technologies.* 2017;12(4):98-105 (in Russ.). https://doi.org/10.32362/2410-6593-2017-12-4-98-105

4. Vichugova A.A. Methods and tools for conceptual design of information systems: comparative analysis of structural and object-oriented approaches. *Prikladnaya informatika* [Journal of Applied Informatics]. 2014;1(49):56-65 (in Russ.).

5. Burlyaeva E., Burlyaev V., Frolkova A. Functional simulation of basic organic synthesis production by vinyl acetate manufacturing. *Khimicheskaya tekhnologiya* [Journal of Chemical Technology]. 2016;9:418-423 (in Russ.).

6. Jeong K.-Y., Wu L., Hong J.-D. IDEF method-based simulation model design and development framework. *Journal of Industrial Engineering and Management.* 2009;2(2):337-359. http://dx.doi.org/10.3926/jiem.v2n2.p337-359

7. Repin V., Eliferov V. Process approach to management. Business process modeling. Moscow: Mann, Ivanov and Ferber Publ., 2013. 544 p. (in Russ.).

8. Maklakov S.V. Business process modeling with All Fusion Process Modeler (BPwin 4.1). Moscow: Dialog-MIFI Publ., 2002. 240 p. (in Russ.).

9. Recommendations for standardization. Information technology support the life cycle of product. Methodology of functional modeling. Moscow: Gosstandart Publ., 2001. 19 p. (in Russ.).

10. Burlyaeva E.V., Burlyaev V.V., Tsekhanovich V.S. Set-theoretic description of functional models of chemical manufacturing. *Tonkie Khimicheskie Tekhnologii = Fine Chemical Technologies.* 2017;12(5):71-78 (in Russ.). https://doi.org/10.32362/2410-6593-2017-12-5-71-78

Список литературы:

1. Черемных С.В., Семенов И.О., Ручкин В.С. Моделирование и анализ систем. IDEF-технологии. М.: Финансы и статистика, 2006. 192 с.

2. Мышенков К.С. Методика обоснования выбора CASE-средств для анализа и проектирования систем управления предприятиями // Инновации. 2013. № 10(180). С. 112–122.

3. Ерушева К.И., Колыбанов К.Ю., Тишаева И.Р. Функциональное моделирование процесса выбора наилучшей доступной технологии // Тонкие химические технологии. 2017. Т. 12. № 4. С. 98–105. https://doi.org/10.32362/2410-6593-2017-12-4-98-105

4. Вичугова А.А. Методы и средства концептуального проектирования информационных систем: сравнительный анализ структурного и объектно-ориентированного подходов // Прикладная информатика. 2014. № 1(49). С. 56–65.

5. Бурляева Е.В., Бурляев В.В., Фролкова А.К. Функциональное моделирование производств основного органического синтеза на примере получения винилацетата // Химическая технология. 2016. № 9. С. 418–423.

6. Jeong K.-Y., Wu L., Hong J.-D. IDEF method-based simulation model design and development framework // J. Ind. Eng. & Manag. 2009. V. 2. № 2. P. 337–359. http://dx.doi.org/10.3926/jiem.v2n2.p337-359

7. Репин В.В., Елиферов В.Г. Процессный подход к управлению. Моделирование бизнес-процессов. М.: Манн, Иванов и Фербер, 2013. 544 с.

8. Маклаков С.В. Моделирование бизнес-процессов с AllFusion Process Modeler (BPwin 4.1). М.: Диалог-МИФИ, 2002. 240 с.

9. Рекомендации по стандартизации. Информационные технологии поддержки жизненного цикла продукции. Методология функционального моделирования. М.: Госстандарт России, 2001. 19 с.

10. Бурляева Е.В., Бурляев В.В., Цеханович В.С. Теоретико-множественное представление функциональных моделей химических производств // Тонкие химические технологии. 2017. Т. 12. № 5. С. 71–78. https://doi.org/10.32362/2410-6593-2017-12-5-71-78

11. Алексеев В.Е., Таланов В.А. Графы и алгоритмы. Структуры данных. Модели вычислений. М.: Интуит, Би-

11. Alekseev V., Talanov V. Graphs and algorithms. Data structures. Calculation models. Moscow: Intuit, Binom Publ., 2012. 320 p. (in Russ.).

12. Markov V.N. Modern logical programming in Visual Prolog 7.5. Saint Petersburg: BHV-Peterburg Publ., 2016. 544 p. (in Russ.).

13. Timofeev V.S., Serafimov L.A., Timoshenko A.V. Principles of technology of basic organic and petrochemical synthesis. Moscow: Vysshaya shkola Publ., 2010. 408 p. (in Russ.).

ном, 2012. 320 с.

12. Марков В.Н. Современное логическое программирование на языке Visual Prolog 7.5. СПб.: БХВ-Петербург, 2016. 544 с.

13. Тимофеев В.С., Серафимов Л.А., Тимошенко А.В. Принципы технологии основного органического и нефтехимического синтеза. М.: Высшая школа, 2010. 408 с.

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Цеханович Виктор Сергеевич, аспирант кафедры информационных систем в химической технологии Института тонких химических технологий им. М.В. Ломоносова ФГБОУ ВО «МИРЭА – Российский технологический университет (Россия, 119571, Москва, пр. Вернадского, д. 86).

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