UDC 628.16:658.512:681.5
DOI: https://doi.org/10.20535/2218-93002522019188250

DESIGN OF SUSTAINABLE INDUSTRIAL WATER NETWORKS: 2. "SEQUENTIAL" SYNTHESIS METHODS.

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Article history:
Received: 1 September 2019
Accepted: 15 October 2019
Print: 20 December 2019

The second part of the work addresses an overview of the modern conceptual methods (also called insight-based, sequential, or hierarchical methods) of project decision support in the sustainable design of water economy networks. The stages of insight-based methods of water economy networks design: graphical/analytic modeling stage to identify the water saving potential as well as optimal network structure synthesis stage were described in detail.

Key words*: design of chemical-engineering systems, water economy, water usage, water treatment, sequential methods, hierarchical methods, pinch analysis, optimization*

Introduction

The first part of this publication was devoted to the review of methods of sustainable design of chemical-engineering systems (CES), in particular, such important subsystem of CES as water economy network (WEN).

As already mentioned in the first part of the article, there are two main classes of CES subsystems sustainable design procedures that deserve the attention: insight-based hierarchical design methods and superstructural simultaneous design methods.

Exhaustive overviews of the WEN conceptual design methods were presented by Foo (2009) (as of February 2009) and also by Jeżowski (2010) – as of early 2010. This paper, therefore, will focus on the following points:

a) a brief description of the principles of the conceptual approach, and

b) consideration of development trends of this approach, which have been defined in recent years.

It should be pointed out that recent review publications in this area are also available (Meng at al. (2014), Venkatesh (2018)). But they largely covered some aspects of industrial implementation of hierarchical design methods.

Main stages of insight-based methods of WEN design

The basic principles of the conceptual approach to WEN design and optimization were formulated by Wang & Smith (1994a, 1994b, 1995). The pre-existing methods of both optimal mass-exchange networks (Hamad & El-Halwagi (1998), El-Halwagi & Manousiouthakis (1990)) and heat-exchange networks (Linhoff & Hindmarsh, 1983) synthesis were successfully used in the development of WEN design ideology. The research vocabulary (including "pinch analysis", etc.) had also been inherited (see, in particular, interesting surveys of the implementation of pinch methodology by Klemes et al., 2018).

Generally "water pinch analysis" (WPA) is a multi-stage procedure that essentially depends on the skill, practical experience and intuition of the researcher.

As it was noted in the first part this paper, the WEN design process involves three phases:

1. Input data preparation.
2. Synthesis of the optimal WEN structure.

3. Preparation for implementation.

When insight-based “water pinch analysis” approach is applied, the phase of the optimal WEN structure synthesis includes the following steps:

Step 1. The “targeting stage”: graphical/analytic modeling of the WEN.

Step 2. Optimal network structure design stage.

Targeting strategies

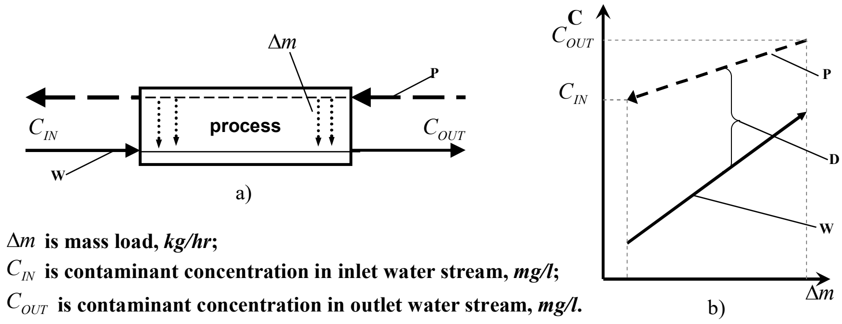
The objective of this stage is to detect the water saving potential (as target) for WEN. In other words, the goal of targeting is to locate minimum permissible values of fresh water consumption as well as wastewater generation.

To fulfill that objective the visual representation (by constructing special-form graphs) of all the WEN constituents is used. An example of such graph/analytic modeling of WEN is the construction of «concentration vs mass load» diagrams.

It should be noted that mass load is expressed as mass transfer per time (see fig. 1). The mass load value can be calculated as follows:

$$\Delta m = f \cdot \Delta C = f \cdot \left(C_{OUT} - C_{IN}\right), \tag{1}$$

where Δm is mass load, f is water flowrate, $\Delta C = \left(C_{OUT} - C_{IN}\right)$ is concentration difference (see fig. 1).



Δm **is mass load,** ***kg/hr*;**

C_{IN} **is contaminant concentration in inlet water stream,** ***mg/l*;**

C_{OUT} **is contaminant concentration in outlet water stream,** ***mg/l*.**

Figure 1 – Concept of water use representation as “concentration vs mass load” diagram: a) water usage process as mass-exchanger; b) – “concentration vs mass load” diagram for a single water usage process; P– «process technology stream»; W – water stream; Δm – mass transferred; D – driving force of mass transfer.

The idea of equation (1) becomes evident from dimensional analysis:

$$\left[\frac{kg\,(of\ cont)}{hour}\right] = \left[\frac{kg\,(of\ cont) + kg\,(of\ water)}{hour}\right] \cdot \left[\frac{kg\,(of\ cont)}{kg\,(of\ cont) + kg\,(of\ water)}\right] \tag{2}$$

For wastewater as dilute solution (2) can be converted as follows:

$$\left[\frac{kg}{hour}\right] = \left[\frac{ton}{hour}\right] \cdot \left[\frac{mg}{litre}\right] \tag{3}$$

In the event that water gains and losses should be taken into account, equation (1) becomes:

$$\Delta m = f_{OUT} \cdot C_{OUT} - f_{IN} \cdot C_{IN} - f_{loss} \cdot C_{loss} + f_{\mathrm{lg}ain} \cdot C_{gain}, \tag{4}$$

where C_{IN} is contaminant concentration in inlet water stream; C_{OUT} is contaminant concentration in outlet water stream; C_{loss} is contaminant concentration in water losses stream; C_{gain} is contaminant concentration in water gains stream; f_{IN} is inlet water stream flowrate; f_{OUT} is outlet water stream flowrate; f_{loss} is water losses stream flowrate; f_{gain} is water gains stream flowrate.

The «concentration vs mass load» mass-transfer representation of water usage process is known in the literature as quality controlled, or fixed load (FL) model.

Example 1. Wang & Smith (1994a) performed the targeting for a simplified WEN (see Table 1), for which the following assumptions were adopted:
a) only water-use mass transfer processes are available (i.e., there are no water treatment as well as water-cooling processes, etc.);
b) there is only one contaminant in the system;
c) water gains and losses are absent;
d) there is only one freshwater source, etc.

Initially, concentration intervals were allocated: the intervals $[0;50]\cup[50;100]\cup[100;400]\cup[400;800]$ correspond to the limiting values of the concentrations (fig 2, a). Next, the "water profiles" of individual water users were built (fig. 2, b). After that, for the network as a whole, the limiting composite curve (fig. 2, c) and also the curve (in the simplest case – the line) of water supply (fig. 2, d) were constructed.

Table 1 – Input data for the WEN synthesis (Wang & Smith, 1994a)

Process number, i	Contaminant mass load, $m_{i,C}$, kg/hr	Limiting concentration of contaminant (process inlet), $C_{i,C\,IN}$, mg/l	Limiting concentration of contaminant (process outlet), $C_{i,C\,IN}$, $C_{i,C\,OUT}$, mg/l
1	2.0	0	100
2	5.0	50	100
3	30.0	50	800
4	4.0	400	800

Water supply line (WSL) begins at the point that corresponds to the contaminant concentration in fresh water. In this case, WSL begins at the origin of the coordinates. The larger the WSL inclination value α to positive direction of mass load axis (abscissa), the lower the freshwater flowrate value. Fig. 2, c shows the limiting case when the angle α is maximal, and the WSL touches the LCC at the pinch point. With a further increase in the angle of WSL inclination, the mass transfer becomes impossible due to the negative driving force of mass transfer. At the pinch point, the driving force of the process is minimal, but not zero. As one can see, the maximum possible angle of inclination of WSL (i.e, the pinch point) corresponds to 90.0 t/hr of freshwater flowrate. Simple calculations indicate that the initial parallel-flow WEN structure is characterized by 112.5 t/hr of freshwater flowrate. That is, due to the synthesis of the optimal WEN 22.5 t/hr of water saving can be achieved.

The diagram shown in fig. 2 was created for the case of water reuse and recycle. As the first approximation, such a diagram can also be used for the network containing water regeneration (i.e., partial treatment of water). But several papers were specifically dedicated to the methods correct calculation of the pinch point for the case of partial wastewater treatment (see, e.g., Kuo & Smith (1998), Feng et al. (2007), Parand et al. (2016), etc.). In particular, Kuo & Smith (1998) used an iterative procedure for interaction between freshwater and water regeneration areas on concentration intervals diagram. Mann & Liu (1999) presented the algebraic "Mass problem table" (MPT) targeting method, which is complementary to limiting composite curves approach from Wang & Smith (1994a).

An essential problem of pinch analysis is taking into account the several contaminants. To achieve this goal Wang & Smith (1994a), Mann & Liu (1999) proposed a so-called "concentration shifting". The method of graphoanalytical formation of the WEN on the basis of the new concept of "water balance" (providing for the construction of "water surplus diagrams" – WSD) was proposed by Hallale (2002). The latter approach is rather difficult to formalize both at the targeting and synthesis stages. However, there are some references to the computer implementation of WSD using so-called “cascade tables” – Water Cascade Analysis (WCA) – see Manan et al. (2004), Wang et al. (2006), Foo et al. (2006), etc.

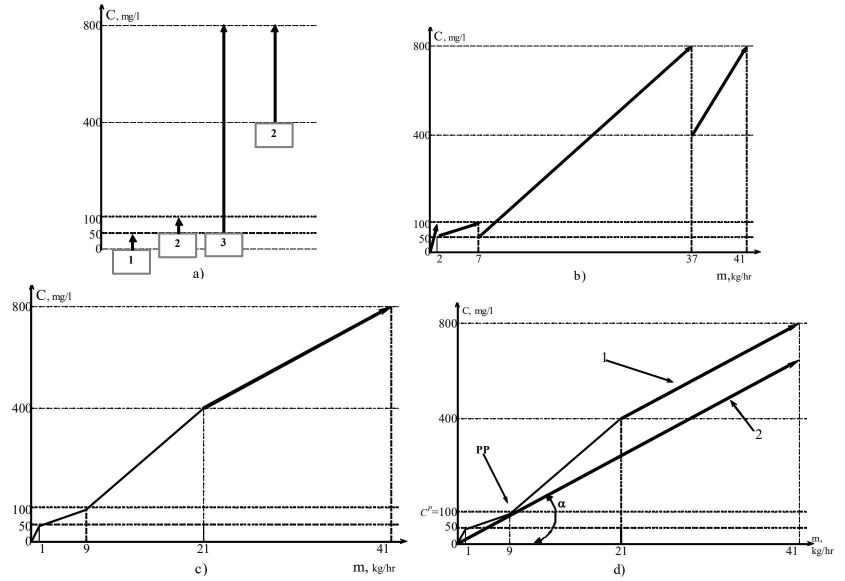


Figure 2 – Graphical/analytic pinch analysis of water usage network (Wang & Smith, 1994a): a) – presenting water users on concentration intervals diagram; b) – graphing water profiles of four individual processes; c) – constructing composite curve, d) – identifying pinch concentration; 1 - limiting composite curve; 2 – water supply line; PP – pinch point.

In certain cases it is possible to group the contaminants according to their properties. In particular, Kutepov et al. (2002) used an integral characteristic of the water contamination (chemical oxygen demand) during the design of WEN of the textile industry. It was hence possible to reduce the problem to the one-contaminant case. After that, the simplest form of water pinch analysis was successfully applied.

As already noted, pinch analysis is quite difficult to formalize, and this hinders attempts to automate WEN design technologies. However, there are some “hybrid” (e.g “algebraic/graphical”) targeting approaches: so-called Composite Table Algorithm (CTA) Agrawal & Shenoy (2006) and also the Source Composite Curve (SCC) method Bandyopadhyay at al. (2006a). The purpose of the Source Composite Curve was to take into account the relationship between water usage and wastewater treatment processes. An analytical model for the pinch point (concentration) determination was proposed by Alva-Argaez et al. (1999) & Jeżowski et al. (2006), who offered to perform pinch analysis using so-called “transshipment model” of linear programming. The mathematical transshipment problem appears as a modification of the classical transportation problem, with taking into account not only the origins (points of production) and destinations (points of consumption), but also intermediate points (warehouses).

The problem of water use is regarded as transportation of contaminant from "technological" flows (i.e., transshipment model’s origins) to water flows (i.e., transshipment model’s destinations) through the concentration intervals (which function as transshipment nodes).

It should be noted that this approach is similar to how energy transportation is considered during the heat-exchange networks design Papoulias & Grossmann (1983), as well as mass transportation is considered during the mass-exchange networks design El-Halwagi & Manousiouthakis (1990). Namely, the “goods” are transported within the intervals of temperature or concentration from "producers" (hot or "rich" streams) to "consumers" (cold or "poor" streams).

The algorithms proposed by Alva-Argaez et al. (1999), Jeżowski et al. (2006) seems to be used not only for a single contaminant, but also for a system of several contaminants (see Pungthong & Siemanond (2015)). The engineering application of these algorithms presented, inter alia, by Nikolakopoulos & Kokossis (2017).

It is also worth mentioning source/sink composite curves or “stream mapping diagrams” (“material recovery pinch diagrams”) approach Dhole et al. (1996), Polley G. & Polley H. (2000), Dunn & Bush (2001), Hallale (2002), El-Halwagi et al. (2003); Prakash & Shenoy (2005), Saw et al. (2011). Source/sink composite curves were built in coordinates «contaminantion vs flowrate» (so-called “water surplus diagrams” – WSD), for example “total suspended solids vs flowrate”. The idea is that WEN is seen not as a set of processes (including water users, water treatment processes, etc.), but as the set of the material (contaminant) sinks and sources. Normally the material sources are outlet streams of water usage processes. Accordingly, units where the resource is consumed are sinks (fig. 4).

Such a way of WEN representation is convenient for WEN containing water users which is not mass-transfer (e.g., chemical reactors using water as reagent, water-steam circuits, chemical facilities as part of eco-industrial parks, some components of urban water networks, etc.).

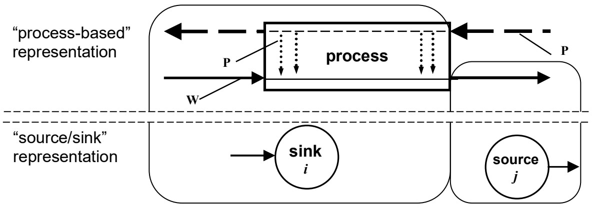


Figure 4 – Concept of material source and sink:
P– «process technology stream»; W – water stream; T – transferable resource (contaminant).

The aim of the «contaminantion vs flowrate» diagrams is to identify various possibilities of single streams interception. The “algebraic targeting” and “improved concentration interval” analysis techniques (Al-Mutlaq et al. (2005), Bandyopadhyay et al. (2006b), Liu et al. (2007a & 2007b)) as well as “automated targeting model” (Ng et al. (2009 & 2014), Bavar et al. (2018)) techniques are computer implementations of source/sink composite curves approach.

The non-mass-transfer representation of water usage process is known in the literature as quantity controlled or fixed flowrate (FF) model.

It should be also noted that there isn’t always one freshwater supply source. There can be several freshwater sources (characterized by different water contamination rates) like mine water, artesian water, etc. And the water sources of “lower quality” are believed to be either free of charge or very cheap. The “multiple utilities” problem was taken into account by “Limiting composite curves” approach (Wang & Smith, 1995), as well as by “Water cascade analysis” (Foo et al. (2006)), and the “Material Recovery Pinch Diagram” approach (Alwi & Manan, 2007), etc. Nevertheless, none of the above contributions adress the “economic efficiency”. Meanwhile, a “cost factor” criterion was proposed by Deng & Feng (2011b) in order to obtain economically optimal combination of water sources used.

Strategies of optimal WEN structure synthesis

At the stage of the network synthesis, all the WEN constituents must be combined in an optimal way to provide optimum flowrates that were calculated at the previous (targeting) stage. It is important to note that network design problems may contain several identical suboptimal solutions and therefore the network synthesis can be recognized as the degenerate problem.

In this regard, the specificity of insight-based approach is the possibility of "step-by-step upgrading" of the sub-optimal structure of the network (see, for example, papers by Ng et al. (2009), Prakash & Shenoy (2005), Wang & Smith (1994a), Li & Chang (2012)). An example of such a "network evolution" is given below (see Example 2).

It should be noted that procedures of WEN structure synthesis differ significantly depending on the type of water users (i.e. either quality controlled (FL) or quantity controlled (FF) problems).

A so-called “water grid diagram approach” was developed by Wang & Smith (1994a) and also by Kuo & Smith (1998), Mann & Liu (1999) for the WEN containing mass-transfer water users (FL problem) – see Example 2.

Olesen and Polley (1997) presented the “Load table” model approach to realize the optimal network structure. Unfortunately, this approach can't deal with more than four (or five) water users as it was based on a special analysis procedure.

Kuo & Smith (1998) also proposed the graphical “Water main method”, under which the “water mains” were identified and then mass balances were made-out in relation to water mains.

Prakash & Shenoy (2005) proposed the heuristics-based approach for design of water network containing FL operations (the “three design rules” approach). Extension of the “three design rules” approach problems can be found in the papers of Deng & Feng (2011a) and Deng et al. (2008).

The “Concentration intervals analysis” approach was proposed by Liu et al. (2007a & 2007b) as the WEN synthesis tool for “Improved concentration interval table method” mentioned above.

Furthermore, such approaches for FL problems as “Mass content diagram” (Mann & Liu, 1999), “Water sources diagrams” (Gomes et al., 2007), etc. were proposed.

Francisco et al. (2015) extended the water source diagram approach by Gomes et al. (2007) to include both FL and FF water users.

Alwi Manan (2007), Parand et al. (2013) provided an original heuristic procedure, which is a modification of the source/sink composite curves approach by El-Halwagi et al. (2003) for the case of several freshwater sources in both quality controlled and quantity controlled problems.

Alwi & Manan (2008) presented “network allocation diagram” (NAD) graphical approach (for quality controlled and quantity controlled problems), which included simultaneous performing both the targeting and synthesis phases.

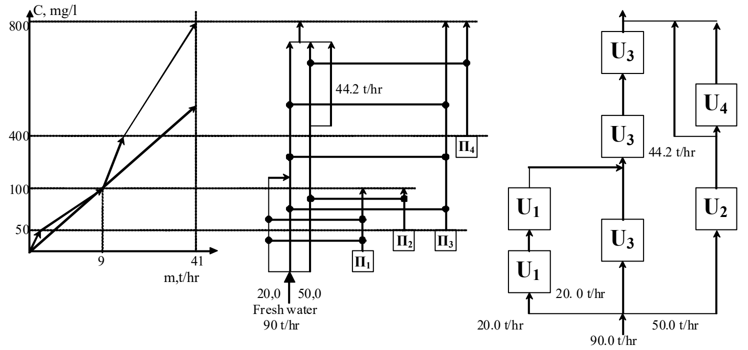
Moreover, such FF-oriented approaches as “Source/demand mapping” Polley G. & Polley H. (2000), “Nearest neighbours algorithm” Prakash & Shenoy (2005), Bandyopadhyay (2006b) “Load problem table” (LPT) Aly et al. (2005) etc. were proposed.

Example 2. The optimal WEN structure must be synthesized on the base of minimum flowrate targets (obtained in example 1), using the following heuristic rules (Wang & Smith, 1994a):

– concentration of contaminant for processes that are “below the pinch concentration C^P” in the pinch analysis diagram, must be increased to pinch concentration value;

– water users, which are “above the pinch point” in the pinch analysis diagram, can not use water with a “less than the pinch concentration C^P” of contaminant concentration

The first step is to construct a design grid (fig. 3, b) based on the water pinch analysis diagram (fig. 3, a).



a) b) c)

Figure 3 – Creating WEN by design grid approach:
a) – limiting composite curve; b) – design grid; c) – initial structure of water usage network;
U_i – water user #i.

The design grid (fig. 3, b) and corresponding WEN structure (fig. 3, c) involves streams mixing “inside” water usage processes. In general, such a technical solution can not be realized. Consequently, the next iteration of the WEN structure creation is required. Wang & Smith (1994a) proposed a loop breaking technique, which eliminates flows bypassing and mixing. fig. 4 shows the loop and the result of the loop breaking procedure.

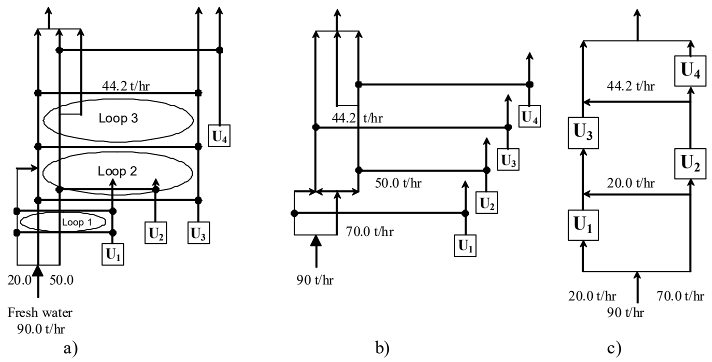


Figure 4 – Loop breaking procedure:
a) – design grid with the loops defined; b) – design grid after loops break; c) – structure of water usage network after loops break;
U_i – water user #i.

As mentioned before, the synthesis routines developed for non-mass-transfer problems are normally unable to handle mass-transfer problems, and vice versa. Nevertheless, Shenoy (2012) proposed an original approach similar to "nearest neighbor algorithm". Note that the above-mentioned algorithm of the nearest neighbor is one of the heuristic methods for solving "travelling salesman problem" (which is one of the common Operation research's problems). The approach of Shenoy (2012) is suitable for solving both quality controlled and quantity controlled problems.

Yet another problem of most water design approaches is the lack of accounting expenses dictated by "plant geography" (i.e the network topology). This problem (relative to WEN) was first formulated in Olesen & Polley (1996). Subsequently, more detailed cost-benefit analysis as part of WEN design process was presented in Alwi & Manan (2006), Rubio-Castro et al. (2010), Aguilar-Oropeza et al. (2019). Some industrial applications of such an approach can be found, e.g., in Parthasarathy & Krishnagopalan (2001), Wenzel et al. (2002), Thevendiraraj et al. (2003), Hamad et al. (2003), Alnouri et al. (2016).

Insight-based methods have a number of advantages. In particular, the visibility of WEN hierarchical design procedures simplifies inclusion sustainable development concepts to the design process. According to this, Ku-Pineda & Tan (2006) proposed a Sustainable Process Index (SPI) to assess the environmental, economic and social implications of implementation of optimized WEN. To address the similar concerns Statyukha et al. (2009) developed a "Water efficiency index" based on the concept of "Life cycle analysis" (LCA). The criterion of the effectiveness of the industrial WEN proposed by Gu et al. (2014), Jia (2015), and Skouteris et al. (2018) is based on the concept of "water environmental footprint". Patole et al. (2016, 2017) applied "Composite quality index", which is based on a set of indicators, including land footprint, carbon footprint, water footprint, inoperability risks, return on energy efficiency investments, etc. The weighting factors for individual indicators are determined by using a well-known hierarchy analysis technique.

Conclusions

A brief analysis of the strengths and capabilities of insight-based methods was performed in this part of the paper.

It has been twenty-five years since the water pinch approach was introduced. Within this time period many of its shortcomings have been eliminated. The visibility of "sequential" design procedures as well as the possibility of taking into account "informal aspects" (e.g. safe conditions of work, aesthetic considerations, etc.), and gathered designers' experience resulted in a significant spread of "water pinch" approach in the design practice.

The third part of the study will consist of an examination of superstructural design methods as alternative approach to sustainable designing of CES subsystems.

Acknowledgments

This paper is respectfully dedicated to the memory of Jacek Jeżowski, Dr.hab. (Ignacy Łukasiewicz Rzeszów University of Technology) and Gennady Statyukha, D.Sc (National Technical University of Ukraine, "Igor Sikorski Kyiv Polytechnic Institute").

The study was conducted within the framework of an ongoing research project "Development of sustainable industrial water networks" (state registration No 0117U005297).

ПРОЕКТУВАННЯ СХЕМ ВОДНОГО ГОСПОДАРСТВА ЗА ПРИНЦИПАМИ СТАЛОГО РОЗВИТКУ: 2. «ПОСЛІДОВНІ» МЕТОДИ СИНТЕЗУ

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Друга частина публікації присвячена огляду сучасних концептуальних методів підтримки прийняття проектних рішень у сталому проектуванні промислових схем водного господарства, тобто технологічних схем водоспоживання, технологічних схем очищення природних та стічних вод. Вказані концептуальні підходи висвітлювалися у літературі також під назвами інтуїтивних, послідовних, ієрархічних методів, тощо.

Задачею статті був аналіз запропонованих у літературі підходів до реалізації концептуальних методів сталого проектування. Було виділено дві базові етапи концептуальних методів проектування – етапи визначення критерію проектування (потенціалу економії води) та синтезу оптимальної схеми водного господарства у відповідності до визначеного раніше критерію проектування. Виконано порівняльний аналіз підходів до визначення потенціалу економії води на основі графічного або графоаналітичного опису промислових схем водного господарства. Показано використання діаграм «масове навантаження – концентрація» для масообмінних процесів водоспоживання (так звані «моделі фіксованого навантаження»), та діаграм «витрата – концентрація» для «немасообмінних» водоспоживачів (так звані «моделі фіксованої витрати»). Показано пропоновані дослідниками шляхи подолання основних недоліків концептуальних підходів – слабкої формалізованості та орієнтованості на досвід технолога-проектувальника, а також методологічних проблем під час розрахунку технологічних схем водоспоживання, очищення природних та стічних вод при врахуванні присутності у воді кількох забруднюючих домішок. Висвітлено характерні особливості та перспективи розвитку евристичних методів синтезу оптимальних схем водного господарств, що забезпечують розрахунковий рівень потенціалу економії води.

Характерні прийоми реалізації концептуальних методів проектування систем водного господарства проілюстровано прикладами.

Ключові слова: *проектування хіміко-технологічних систем, водне господарство, водоспоживання, очищення води, послідовні методи, ієрархічні методи, пінч-аналіз, оптимізація*

ПРОЕКТИРОВАНИЕ СХЕМ ВОДНОГО ХОЗЯЙСТВА В СООТВЕТСТВИИ С ПРИНЦИПАМИ УСТОЙЧИВОГО РАЗВИТИЯ: 2. «ПОСЛЕДОВАТЕЛЬНЫЕ» МЕТОДЫ СИНТЕЗА.

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Вторая часть публикации посвящена обзору современных концептуальных методов (известных также под названиями интуитивных, последовательных, иерархических методов) поддержки принятия проектных решений в устойчивом проектировании промышленных схем водного хозяйства, то есть схем водопотребления, схем очистки природных и сточных вод.

Проанализированы предложенные в литературе подходы к реализации концептуальных методов устойчивого проектирования как на стадии определения цели проектирования – потенциала экономии воды (путем графического или графоаналитического описания промышленных схем водного хозяйства), так и на стадии синтеза оптимальной схемы водного хозяйства.

Ключевые слова: *проектирование химико-технологических систем, водное хозяйство, водопотребление, очистка воды, последовательные методы, иерархические методы, пинч-анализ, оптимизация*

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