

Mass Integration of a Large-Scale Gas Oil Hydrocracking Process using Pinch Analysis

Sofía García-Maza, Luisa J. Acosta-Esalas, Ángel D. González-Delgado*

Chemical Engineering Department, Nanomaterials and Computer-Aided Process Engineering Research Group (NIPAC), Universidad de Cartagena, Cartagena 130014, Bolívar, Colombia.
agonzalezd1@unicartagena.edu.co

Gas oil hydrocracking has improved refinery economics; however, its high water consumption has generated efforts to mitigate its environmental impact. Using wastewater reduces industrial requirements, freeing up more water for communities and decreasing the use of natural resources. For this reason, in this work, the mass integration of an energy-integrated hydrocracking plant is proposed based on process simulation, considering the general conditions of the system and the extended development of the material and energy balances, using the Aspen HYSYS® simulator, the mass-Pinch analysis methodology and mathematical optimization. The results show that for a loading capacity of 61.43 kg/s of gas oil, 58.83 kg/s of products were obtained, including LPG (liquefied petroleum gas), diesel, kerosene, light naphtha, and heavy naphtha. Finally, it was determined that 10.16 kg/s of wastewater is generated in the process, which is reduced to 7.59 kg/s after mass integration. These results demonstrate that the conventional gas oil hydrocracking process supports the mass integration of water effluents, obtaining a saving percentage of 25.54 % of freshwater.

1. Introduction

Water is one of the most crucial natural resources on the planet, covering approximately 70 % of its surface, of which 97.5 % is salt water and 2.5 % is freshwater. However, only freshwater is the most suitable for consumption, and its access is becoming increasingly limited due to global warming, pollution, and intensive use in productive activities, such as industry (Gosling et al., 2011). This is generating preoccupation in growing human populations that face difficulties in meeting their daily needs, such as food, which causes social and economic problems worldwide (Teh and Wu, 2014). On the other hand, the global economy is highly dependent on the supply of petroleum-derived fuels, which are limited, environmentally harmful, and potentially unstable resources (Gebresslassie et al., 2013). In this sense, one of the processes that depends on these non-renewable resources is gas oil hydrocracking, which in recent years has received increasing attention from oil refining industries, especially in the context of digitalization (Iplik et al., 2020). This is due to the prevailing demand for middle distillates such as kerosene and diesel, particularly in developing countries, and the growing emphasis on the production of environmentally clean transportation fuels (Bhan et al., 2020). Accordingly, hydrocracking is a very suitable process due to its ability to convert heavy and/or sulfur- and aromatic-rich feedstocks, like gas oil, into high-quality middle distillate products, i.e., low in sulfur and aromatics, with excellent combustion properties, like diesel, kerosene, and gasoline (Song et al., 2017).

According to the use of available industrial resources, in the conventional gas oil hydrocracking process 36.24 m³/h of demineralized water is used for washing, stripping, and fractionation processes, of which 77.61 % ends up as wastewater; this value is considered high compared to what would be expected and indicates that water resources are not being used in a sustainable manner, which harms the environment, consumption in the surrounding communities and the internal economy of the process. This is the main problem within the limits of the gas oil hydrocracking process, which is presented to be solved without including external processes, such as the production of hydrogen that feeds the hydrocrackers. Therefore, it is necessary to develop a mass integration process, specifically the recirculation of wastewater effluents, similar to the methodology applied in the research developed by Mughees and Al-Ahmad (2015), where mass integration was carried out with mass-

Pinch analysis to reduce water consumption and wastewater emission for a refinery that consumes 505 m³/h. This study can be considered as a precedent for current research.

In modern times, water resource productivity in industry is an indicator of the efficiency with which a country uses its water resources (Yessymkhanova et al., 2021). For this reason, it is necessary to reduce the consumption of freshwater in the gas oil hydrocracking process, which the recirculation of the sour waters of the process after its adequate treatment is proposed. In this sense, it is proposed to carry out a mass integration of wastewater effluents with direct recycling under the criterion of a single limiting pollutant, applying the Pinch analysis approach using the graphical method of accumulated loads to determine the Pinch point, the minimum target amount of freshwater and wastewater in the process, as well as the percentages of savings in freshwater and wastewater, and the configuration of the network (Ongpeng et al., 2019). A study similar to that developed by González-Delgado et al. (2023) regarding the industrial-scale production of bioadsorbents from chitosan modified with iron nanoparticles and functionalized with thiourea as a chelating agent. It was concluded that mass integration reduced up to 51 % of the freshwater used in the processes.

The implementation of gas oil hydrocracking technology has enhanced refinery economics but raised environmental concerns due to its high consumption of water, energy, and raw materials. Addressing these issues involves optimizing process flows to reduce industrial demands, making more water and energy available for residential use, and conserving natural resources. This highlights the importance of specialized computational tools to optimize industrial processes, minimize water footprints, and promote sustainable practices. This study focuses on the mass integration of an energy-integrated hydrocracking plant using process simulation, employing Aspen HYSYS[®], mass-Pinch analysis, and mathematical optimization to develop material and energy balances under system-specific conditions.

2. Materials and methods

2.1 Global process description

The mass and energy-integrated gas oil hydrocracking process retains the key stages of the base case presented by García-Maza and González-Delgado (2024), i.e., it includes a reaction stage, where the conditioning of the feedstock and the hydrotreating and hydrocracking reactions in the hydrocrackers occur; a preliminary separation stage, in which the process is separated into high and low-pressure sections using flash evaporators and the main process contaminants (ammonia, NH₃, and hydrogen sulfide, H₂S) are removed through three-phase separators, lean amine scrubbing towers, and PSA stage; a make-up and recycling gas (hydrogen) stage to regulate the operating conditions of the fresh hydrogen entering the process and mix with the recycled hydrogen; a stripping stage to separate the heavy components from the light ones; a debutanization stage, where LPG is produced; a fractionation stage to produce diesel and kerosene; and a naphtha separation stage, in which light and heavy naphtha are produced. However, previously integrated energetically, it should be noted that the process has an additional stage of make-up freshwater and recirculation of sour water effluents, where the wastewater generated in the stages of preliminary separation, stripping, debutanization, fractionation, and naphtha separation ends up.

2.2 Mass integration with Pinch methodology

The problem of high water consumption for the conventional gas oil hydrocracking process through direct wastewater recycling networks without removal of contaminants under the criterion of a single limiting contaminant per sink is analyzed, similar to the research developed by Moreno-Sader et al. (2021) on an integrated biorefinery approach through material recycling/reuse networks for the extraction of value-added components from shrimp. The graphical technique proposed by El-Halwagi et al., (2003) was selected to locate the Pinch point and determine the minimum use of fresh resources and the minimum discharge of waste. First of all, information related to the initial consumption of freshwater and acidic water effluents was obtained from the simulation of the conventional process. Then, the sources and sinks of the process were determined, where the former are related to wastewater and the latter to the stages of the process that require water feed. The compositions of the two pollutants present in the sources and sinks of the process (NH₃ and H₂S) were established, selecting the critical pollutant in each sink under the minimum ratio criterion using Eq(1), and consequently, the system will be oriented through a single-pollutant approach (González-Delgado et al., 2023). Additionally, the percentages of savings in fresh and residual water were calculated after carrying out the mass integration with the Pinch methodology using the graphical method of accumulated loads and determining the Pinch point, the minimum freshwater requirements, and the minimum acidic water effluents. Finally, the network configuration was carried out with mathematical optimization where the source and sink pairs and the amount of freshwater that feeds each sink were determined; taking into account that when considering the reuse of water between operations, a water network must be designed that meets the concentration requirements of the critical contaminant (Cortés et al., 2011).

$$\frac{Z_{*k,skj}}{C_{*k,sr_max}} = \frac{Z_{k,skj} - C_{k,FW}}{C_{k,sr_max} - C_{k,FW}} \quad (1)$$

Where, $Z_{*k,skj}$ is the difference between the fraction of pollutant k in sink j and the fraction of pollutant k in freshwater (FW), $Z_{k,skj}$ is the fraction of pollutant k in sink j, $C_{k,FW}$ is the fraction of pollutant k in freshwater (FW), and C_{k,sr_max} is the maximum fraction of pollutant k in sources.

2.3 Computer-aided process simulation

The mass integration simulation of the energetically integrated gas oil hydrocracking process was conducted using Aspen HYSYS®, a widely used simulator in the oil and gas industry (Nekrasov et al., 2023). Conventional components available in the simulator were selected, avoiding hypothetical components or a predefined feed. Suitable fluid packages, including state equations and solution models, were chosen for each process stage. The simulation incorporated various equipment types, such as hydrocrackers, distillation columns, flash evaporators, separators, mixers, heat exchangers, air coolers, ovens, pumps, compressors, and valves. The HYSYS recycling function was used to optimize mass integration and ensure convergence. The simulation results provided material and energy balances for the processes. Finally, the simulation was validated by comparing it with real plant data.

3. Results and discussion

3.1 Mass integration of the gas oil hydrocracking process

Tables 1 and 2 summarize the sinks and sources of the gas oil hydrocracking process that were selected focusing on the washing, stripping, and fractionation stages for the sinks, while for the sources of the wastewater from three-phase separators in the preliminary separation section, and top drums in the stripping, debutanization, fractionation, and naphtha separation stages were selected. The mass flows of the streams for the 5 sources and the 4 sinks can be observed, as well as the total mass flows (10.1601 kg/s for the sources and 10.0679 kg/s for the sinks), the concentration of the main process pollutants, NH₃ and H₂S, and the load for both pollutants. Using Eq(1) it was determined which of the two main pollutants is the one that limits the mass integration, considering the minimum ratio. The results of this calculation are shown in Table 3, where it is shown that the minimum ratio (0.085) is obtained by ammonia (NH₃), while H₂S obtains a higher ratio (0.1). In this particular case, the physicochemical characteristics that must be taken into account in wastewater are those related to the ammonia concentration, which is the critical pollutant.

Table 1: Source data for the gas oil hydrocracking process.

Source	Description (water from)	Flow rate (kg/s)	Mass fraction NH ₃	Mass fraction H ₂ S	Load NH ₃ (kg/s)	Load H ₂ S (kg/s)
SR1	Naphtha Separator (T-107)	0.0088	0.00	0.000	0.00000	0.000000
SR2	Fractionator (T-106)	1.0707	0.00	0.000	0.00000	0.000000
SR3	Debutanizer (T-103)	0.0003	0.02	0.002	0.00001	0.000001
SR4	Stripper (T-102)	1.1559	0.01	0.001	0.01147	0.001156
SR5	LLV Separator (V-104)	7.9245	0.02	0.000	0.12586	0.000000
Total		10.1601				

Table 2: Sink data for the gas oil hydrocracking process.

Sink	Description (water for)	Flow rate (kg/s)	Mass fraction NH ₃	Mass fraction H ₂ S	Max inlet load NH ₃ (kg/s)	Max inlet load H ₂ S (kg/s)
SK1	Fractionator (T-104)	1.0802	0.0000	0.0000	0.000	0.0000
SK2	Stripper (T-102)	1.1296	0.0000	0.0000	0.000	0.0000
SK3	Washing 2 (MIX-107)	0.7787	0.0020	0.0002	0.002	0.0002
SK4	Washing 1 (MIX-106)	7.0794	0.0020	0.0002	0.014	0.0014
Total		10.0679				

Table 3: Critical contaminant selection from the gas oil hydrocracking process.

Sink	$Z_{NH_3}/C_{NH_3,max}$	$Z_{H_2S}/C_{H_2S,max}$	Minimum ratio	Key contaminant
SK1	0.000	0.000	-	-
SK2	0.000	0.000	-	-
SK3	0.085	0.100	0.085	NH ₃
SK4	0.085	0.100	0.085	NH ₃

Figure 1 shows the cumulative load graph of sources and sinks, from which the Pinch point (black dot on the graph), the minimum amount of freshwater, FW (7.50 kg/s) entering the process and the minimum amount of wastewater, WW (7.59 kg/s) leaving as effluents from the process can be located. Additionally, Figure 2 shows the configuration network diagram, where the pairings between sources and sinks, the amount of freshwater feeding each sink and the amount of sour water leaving the mass-integrated gas oil hydrocracking process are established. As it was mentioned in section 2.2, these results were obtained by applying mathematical optimization where the source-sink pairs and the amount of fresh water that feeds each sink were determined. The amount of freshwater fed to the process is distributed among the four sinks of the process; 1.08 kg/s is fed to sink 1 (fractionator), 1.13 kg/s to sink 2 (stripper), 0.61 kg/s to sink 3 (wash 2), and 4.67 kg/s to sink 4 (wash 1). Sources 1 (naphtha separator) with 0.01 kg/s, 3 (debutanizer) with 0.0003 kg/s, and 4 (stripper) with 1.16 kg/s feed only sink 4. While sources 2 (fractionator) and 5 (three-phase separator in the preliminary separation stage) are distributed between sink 3 and sink 4; source 2 provides 0.05 kg/s to sink 3 and 1.02 kg/s to sink 4, and source 5 provides 0.11 kg/s to sink 3 and 0.22 kg/s to sink 4. Additionally, after integration, a savings of 25.54 % was achieved for freshwater and 25.31 % for wastewater.

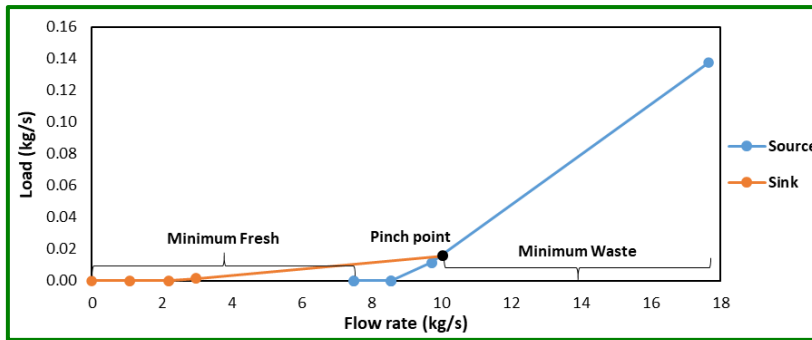


Figure 1: Accumulated load chart of sources/sinks of the gas oil hydrocracking process.

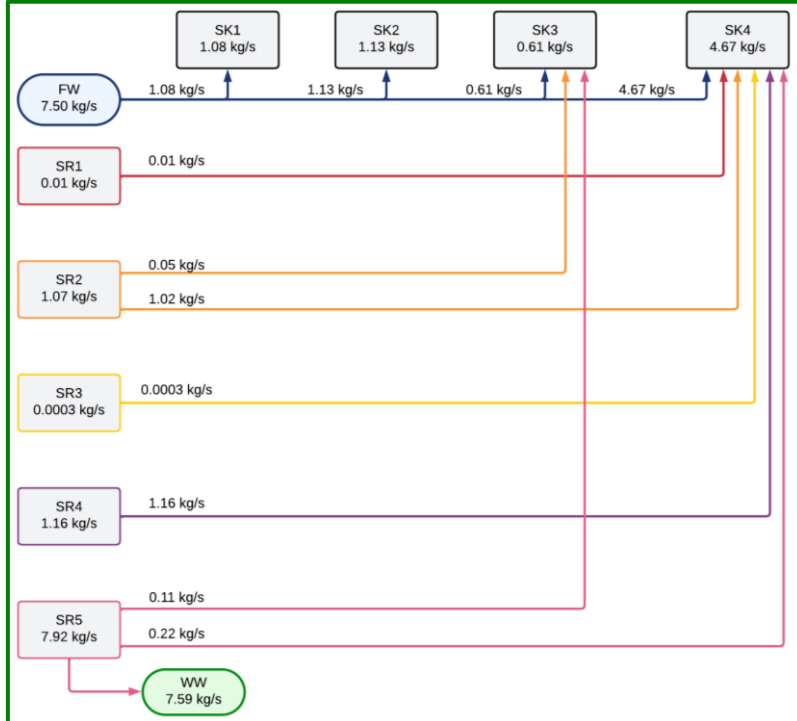


Figure 2: Network configuration diagram of the mass-integrated gas oil hydrocracking process.

In this sense, direct recycling of wastewater in real refineries significantly reduces freshwater consumption by allowing wastewater to be immediately reused within industrial processes. Unlike indirect recycling, which

requires external treatment, direct recycling minimizes water losses and energy use associated with additional treatment steps including ultrafiltration, chemical treatment, and reverse osmosis. By optimizing direct recycling of wastewater, refineries can improve water conservation, reduce operating costs, and reduce environmental impact (Maheshwari et al., 2019).

3.2 Process simulation for the mass and energy-integrated gas oil hydrocracking process

Figure 3 shows the simulation results for the mass and energy-integrated gas oil hydrocracking process. The main process feedstock is a load of gas oil (61.43 kg/s at 112 °C and 446 kPa) and the principal product is diesel (29.61 kg/s at 43 °C and 203 kPa). Furthermore, after implementing mass integration, the process reduces wastewater generation from 10.16 kg/s to 7.59 kg/s. Additionally, the process operates continuously and exhibits an overall energy consumption of 3,130 GJ/h, of which 19 GJ/h is used in the reaction stage, 1,838 GJ/h in the preliminary separation, 96 GJ/h in the make-up and recycle gas stage, 0.66 GJ/h in the PSA, 237 GJ/h in the stripping, 8 GJ/h in the debutanization, 884 GJ/h in the fractionation, 48 GJ/h in the naphtha separation, and 0.55 GJ/h in the make-up and recycle water stage. It's necessary to present the entire diagram considering that mass integration was performed for the whole unit.

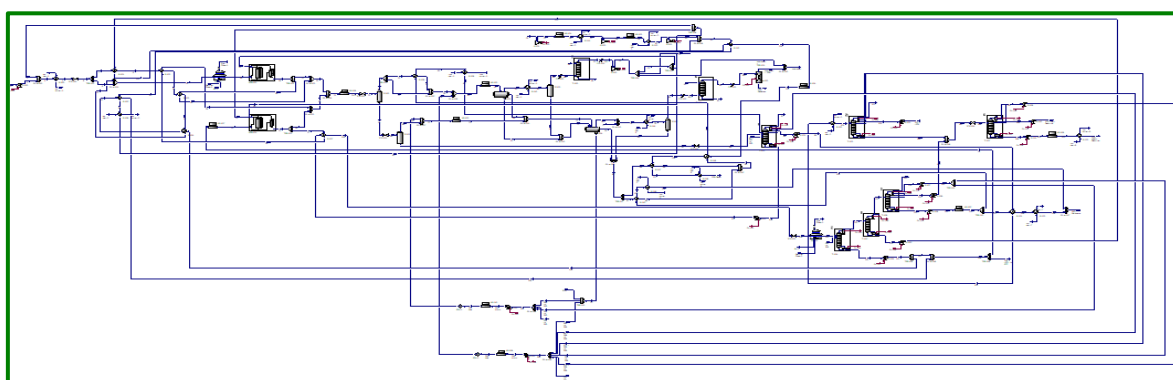


Figure 3: Simulation of the mass and energy-integrated gas oil hydrocracking process.

Table 4 validates the simulation by comparing its results with the literature data (National Institute of Standards and Technology (NIST), 2023), confirming high accuracy in predicting thermophysical properties of LPG, diesel, and kerosene. The analysis, based on industry reports and pilot plant experiments, shows that the simulation achieves over 94 % accuracy under standard conditions.

Table 4: Validation of the simulation of the mass and energy-integrated gas oil hydrocracking process.

Variable	Literature	Simulation	Accuracy
Diesel viscosity (Pa.s)	0.0024 – 0.0032	0.00242	99.17 %
LPG higher heating value, HHV (kJ/kg)	49,299.57 – 55,200.63	48,765.40	98.92 %
Kerosene density (kg/m ³)	768.89 – 832.96	724.35	94.21 %

4. Conclusions

The mass-integration of an energy-integrated gas oil hydrocracking process was analyzed using the Aspen HYSYS® simulator in combination with mass-Pinch analysis methodology and mathematical optimization techniques. The study considered a gas oil loading capacity of 61.43 kg/s, resulting in a product output of 58.83 kg/s. Through the implementation of mass integration strategies, significant improvements in water usage efficiency were achieved. Specifically, the minimum freshwater intake required for the process was reduced from 10.07 kg/s to 7.50 kg/s, while the minimum wastewater discharge decreased from 10.16 kg/s to 7.59 kg/s. These reductions translate into considerable water savings, with freshwater consumption decreasing by 25.54 % and wastewater effluent generation lowering by 25.31 %. The optimization of the process through the strategic combination of sources and sinks ensured a more efficient use of available water resources. As a result, the hydrocracking process not only improved its sustainability by minimizing environmental impact but also enhanced technical performance. The reduction in freshwater demand and wastewater production benefits both industrial operations and the surrounding communities by preserving natural water sources, lowering treatment costs, and promoting environmentally responsible practices in oil refining.

Nomenclature

$C_{k,FW}$ – fraction of pollutant k in FW	SK – sink
$C_{k,SR_{max}}$ – max. fraction of pollutant k in sources.	SR – source
FW – freshwater	WW – wastewater
HHV – higher heating value	$Z_{*k,skj}$ – difference between $Z_{k,skj}$ and $C_{k,FW}$
LPG – liquefied petroleum gas	$Z_{k,skj}$ – fraction of pollutant k in sink j

Acknowledgments

The authors thank the Universidad Cartagena for funding this research presented in the twelfth call for visible research groups (categorized or recognized) on the Scienti platform of the Ministry of Sciences, Technology, and Innovation by Resolution No. 00470 of 8 March 2022, approved by Resolution 01880 of 2022 and commitment act No. 027 of 2022.

References

- Bhan, C., Verma, L., Singh, J., 2020, Alternative fuels for sustainable development, *Environmental Concerns and Sustainable Development: Volume 1: Air, Water and Energy Resources*, 317–331.
- Cortés, M. G., Verelst, H., Pedraja, R. E., Suárez, E. G., 2011, Simultaneous energy and water minimization applied to sugar process production, *Chemical Engineering Transactions*, 25, 177–182.
- El-Halwagi, M. M., Gabriel, F., Harell, D., 2003, Rigorous graphical targeting for resource conservation via material recycle/reuse networks, *Industrial & Engineering Chemistry Research*, 42(19), 4319–4328.
- García-Maza, S., González-Delgado, Á. D., 2024, Robust simulation and technical evaluation of large-scale gas oil hydrocracking process via extended water-energy-product (E-WEP) analysis, *Digital Chemical Engineering*, 13, 100193.
- Gebreslassie, B. H., Slivinsky, M., Wang, B., You, F., 2013, Life cycle optimization for sustainable design and operations of hydrocarbon biorefinery via fast pyrolysis, hydrotreating and hydrocracking, *Computers & Chemical Engineering*, 50, 71–91.
- González-Delgado, Á. D., Cogollo-Cárcamo, G., Bertel-Pérez, F., 2023, Mass-Integration and Environmental Evaluation of Chitosan Microbeads Production Modified with Thiourea and Magnetite Nanoparticles, *Processes*, 11(7).
- Gosling, S. N., Arnell, N. W., Lowe, J. A., 2011, The implications of climate policy for avoided impacts on water scarcity, *Procedia Environmental Sciences*, 6, 112–121.
- Iplik, E., Aslanidou, I., Kyprianidis, K., 2020, Hydrocracking: A perspective towards digitalization, *Sustainability*, 12(17), 7058.
- Maheshwari, A., Prasad, V., Gudi, R. D., Biswas, P., 2019, Systems engineering based advanced optimization for sustainable water management in refineries, *Journal of Cleaner Production*, 224, 661–676.
- Moreno-Sader, K. A., Martínez-Consuegra, J., González-Delgado, Á. D., 2021, An integrated biorefinery approach via material recycle/reuse networks for the extraction of value-added components from shrimp: Computer-aided simulation and environmental assessment, *Food and Bioprocess Processing*, 127, 443–453.
- Mughees, W., Al-Ahmad, M., 2015, Application of water pinch technology in minimization of water consumption at a refinery, *Computers & Chemical Engineering*, 73, 34–42.
- National Institute of Standards and Technology (NIST), 2023, *The NIST Chemistry WebBook*.
- Nekrasov, I., Tynchenko, V., Bukhtoyarov, V., Panfilova, T., Sokolnikov, A., Gorodov, A., Panfilov, I., 2023, Simulation of the hydrocracking process to produce diesel fuel in the aspen hysys system, *AIP Conference Proceedings*, 2700.
- Ongpeng, J. M. C., Aviso, K. B., Foo, D. C. Y., Tan, R. R., 2019, Graphical pinch analysis approach to cash flow management in engineering project, *Chemical Engineering Transactions*, 76, 493–498.
- Song, W., Zhong, W., Yang, M., Du, W., Qian, F., 2017, A new lumped kinetic model of an industrial hydrocracking process, *Chemical Engineering Transactions*, 61, 673–678.
- Teh, C. Y., Wu, T. Y., 2014, The potential use of natural coagulants and flocculants in the treatment of urban waters, *Chemical Engineering Transactions*, 39, 1603–1608.
- Yessymkhanova, Z., Dauletkanova, Z., Suleimenova, B., Mussirov, G., Gorda, A., Gorda, O., Kolesnikova, E., Niyazbekova, S., Maisigova, L., 2021, The potential of the water industry in the context of sustainable development, *IOP Conference Series: Earth and Environmental Science*, 937(3), 032027.