AI and BD in Process Industry: A Literature Review with an Operational Perspective

Rosanna Fornasiero, David F. Nettleton, Lorenz Kiebler, Alicia Martinez de Yuso, Chiara Marco

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Rosanna Fornasiero[1[0000-0002-7198-2254]], David F. Nettleton[2[0000-0002-5852-7716]], Lorenz Kiebler[3[0000-0002-7348-4611]], Alicia Martinez de Yuso[4[0000-0001-8493-9784]] and Chiara Eleonora De Marco[5[0000-0003-3151-3768]]

[1] CNR-IEIIT, Via Gradenigo, 6, 35100 Padova, Italy
rosanna.fornasiero@ieiit.cnr.it
[2] IRIS Technology Solutions S.L., Ctra. d'Esplugues, 39-41, 08940 Cornellà de Llobregat, Barcelona, Spain
david.nettleton@iris-eng.com
[3] Fraunhofer Institute for Material Flow and Logistics IML, Joseph-von-Fraunhofer-Str. 2-4, Dortmund, Germany
lorenz.kiebler@iml.fraunhofer.de
[4] Zaragoza Logistics Center, Zaragoza, Spain
amartinez@zlc.edu.es
[5] CiaoTech s.r.l. – PNO Group, Italy
C.DeMarco@ciaotech.com

Abstract. Among digital technologies, Artificial Intelligence (AI) and Big Data (BD) have proven capability to support different processes, mainly in discrete manufacturing. Despite the fact that a number of AI and BD literature reviews exist, no comprehensive review is available for the Process Industry (i.e. cements, chemical, steel, and mining). This paper aims to provide a comprehensive review of AI and BD literature to gain insights into their evolution supporting operational phases of the Process Industry. Results allow to define the areas where AI/BD are proven to have greater impact and areas with gaps like for example the process control (predictive models) area, machine learning and cyber-physical systems technologies. The sectors lagging behind are Ceramics, Cement and non-ferrous metals. Areas to be studied in the future include the interaction between intelligent systems. humans and the external environment, the implementation of AI for the monitoring and optimization of parameters of different operations, ethical and social impact.

Keywords: Operations management, Artificial Intelligence, Big Data, process industry.

1 Introduction

In the recent years, the great potential of AI/BD has enabled firms to increase their profits and 85% of business leaders believes that these technologies will make their businesses remain competitive. Adoption rates are still quite low, around only 23% adopting some AI/BD technology and a mere 5% having extensively deployed AI/BD solutions and mostly in support functions such as IT and customer service [1]. Nonetheless, 77% of industry managers considered machine learning to be most useful in deploying AI, with smart robotics second (44%), natural language processing third (40%).

Concerning BD, businesses are rapidly growing the volume of their owned digital data, generated from different sources and in different structures, by increasing the amount of users, sensors, processes and other sources. In many cases, BD is a prerequisite of AI, as it goes beyond traditional database software tools, to enable access, storage, management of large amounts of data to be analysed, interpolated and correlated in AI applications. Important issues for AI are the data collection, access and processes therefore very much in relation with BD handling. Therefore, a high data quality and availability and the implementation of the right algorithms and learning processes, are the biggest challenges for AI [2]. While Process Industry already generates a vast amount of data, it is still facing the challenge of integrating and define data structures and interfaces to create a common access over several processes and locations for usage at operational level by means of AI. In other cases, process industry do not have capability to gather this data available to apply machine learning techniques in a suitable way.

Several papers demonstrate that in discrete manufacturing companies AI/BD technologies can improve performance in terms of efficiency, sustainability, flexibility, agility, robustness and resilience. In the case of the Process industry, the application of AI/BD is lagging behind given the differences in operations (continuous flows can have different problems in terms of monitoring and control with respect to discrete production) and only recently has started to adopt these technologies. The aim of this paper is to conduct a literature review to analyse to what extent AI/BD are used at different operational levels in the process industry to transform data, facilitate real-time decision making using online data and automate decision making. After the presentation of the methodology and the AI/BD taxonomy, the paper proposes a structured analysis of available works in AI/BD fields applied to eight sectors of the Process Industry namely cement, ceramics, chemicals, engineering, minerals and ores, non-ferrous metals, steel, water. As part of the synthesis, on the one hand, the operations which show most important applications of technologies are identified, and on the other, gaps are detected for further study and evaluation.

2 Methodology and AI /BD taxonomy

The literature review (LR) is recognized as a valid approach and a necessary step for exploring new directions guiding the research toward identifying research gaps and proposing innovative applications with cross-sectorial comparison. A four-step process proposed by [3] was adopted:

1. *Material collection*: based on the research scope, the collection of papers and scientific contributions was carried out by using the search engine of Web of Knowledge and google scholar. A publication search was conducted in terms of structured combination of the key words in title, abstract and keywords taking into consideration technologies as defined in the taxonomy and the process industry sectors. Since

one of the main objectives is to analyse the recent developments of AI and BD, the search was limited to the last 5 years.

2. *Descriptive analysis*: more than 300 papers have collected and analysed by the partners of the project and a preliminary analysis of the formal aspects was used to assess the material in a qualitative way. During the material revision, some references were discarded and other were found of interest and added to our LR. Totally around 200 papers have been kept for categorisation. For reasons of space, in this paper we report only a subset of the most important papers. The full list is available upon request.

3. *Material categorisation*: the collected papers were categorised according to the involved operational dimensions and coded accordingly to obtain a picture of the use of the AI/BD technologies in the eight sectors.

4. *Analysis and results*: during the analysis particular attention have been given to how AI/BD can support processes, establishing which are the most important operations where these technologies can be implemented.

Before to start the LR, a taxonomy has been developed specifically for the AI-CUBE project [4] taking into account current state of the art taxonomies, including the one developed by the EC AI Expert group [5], which has been customized for process industries. In particular, the AI taxonomy has two core categories, "perception and communication" and "cognition and reasoning" and one transversal category "integration and interaction". From these, nine sub-categories are identified, which are summarized and five categories for BD.

Table 1. Taxonomy for AI/BD

Category	Technology	Acronym
AI- Perception and communication	Data understanding and characterization	DUC
	Natural language processing	NLP
	Object and spatial recognition	OSR
	Machine learning	ML
AI- Cognition and reasoning	Intelligent planning	IP
	Expert systems	ES
	Case based reasoning	CBR
AI- Integration and interaction	Intelligent agents	IA
	Cyber-physical systems	CPS
BD –Big Data	Data visualisation	DV
	Data processing	DP
	Data protection	DPR
	Data management	DM
	Computing and storage infrastructure	CSI

3 Results

Steel sector: there are several examples of ML used for different processes as for example for fatigue property analysis [6] and to predict the tensile strength of steel rods manufactured in an electric arc furnace [7]. ML is also used to enable prediction of systems failure [8] and neural network-based solutions are used for crack prediction to improve the steel-casting process. ES have been developed to analyse the quality of the steel products [9] and for the analysis of metallurgical processes related to continuous casting with a modular system architecture while the DM system is based on the physical and chemical features of steel [10]. NLP is used for entity recognition for the steel product categories; while for OSR, vision-based automatic identification can track without embedding identification codes onto the steel product surfaces [11]. CPS and knowledge-based systems are used to detect functional failure to reduce the time of expertise acquisition and the cost of solving over-generalization and over-fitting problems with a data driven tool to provide fault diagnostics enabling risk-informed decision-making [12].

Engineering sector: NLP can be integrated in various processes along the value chain, as in the automated mapping of the SC based on text sources for archiving visibility [13] or in the extraction of satisfactory product properties from customer reviews [14] for a customer-centric product customization. ML can be used along the whole process, for example in data driven models for characterising engineering systems [14]. An exemplary field of application for frameworks and systems of intelligent agents can be to address systems engineering problems [15]. In particular, CPS are often used for proactive or predictive maintenance solutions and tools, as described in [16]. Other predictive maintenance solutions can be based on BD like DM and DP, for example by using digital twins [17]. DV for value analysis [18] is also considered.

Ceramics: ML is applied for quality control in the ceramics industry for the detection and classification of defects in the final product in combination with other technologies, like ultrasound sensing [19]. IS using ML (ANN) for the analysis of acoustic emissions and cutting power signals [20] have been applied to predictive maintenance. IP is used for quality control in the manufacturing process, i.e. trajectory planning system solution for glazing spraying using cooperative multi-robots [21] and to optimize experimental conditions to obtain maximum hardness of ceramic samples [22]. Optimization, classification and processing, for example in evaluating rotary ultrasonic machining to select optimum machining parameters can be based on ES [23], while OSR has been applied for Additive Manufacturing technologies for optimization of process, and [24] reported the development of a new feature-based method for identification of geometric features and manufacturing constrains. The development of smart ceramic manufacturing is based on the interconnection assured by with CPS [25] or through IoT based BD analytics [26].

Minerals: [27] main operations in reaching the ore, breaking the ore underground to bring it to the surface and then dressing and smelting it can be supported by AI as a lead technology in decision-making. BD and ML can improve operational efficiency, mine safety, and production workflow [28]. Key operational areas for leveraging from AI are cited as mineral processing and exploration, safety/security, and autonomous vehicles and drillers (SLAM technology). Current issues/problems in the sector include: milling of raw material, mining / extraction, high energy consumption, security and human safety, scheduling / planning, security, automation and remote monitoring.

Cement: being an energy-intensive sector, innovative approaches based on AI/BD can help to reduce energy consumption and costs in this sector supporting new strategies for optimization of usage. In [29] an AI model (deep learning neural network) learns the dynamics of each of the key industrial assets (cooler, ball mill, vertical mill, pre-heater, and kiln) and processes from historical sensor data, creating prescriptions by searching for the optimal values of critical control parameters. Moreover, there are some operational phases that need to be supported by AI/BD like kiln, firing, material processing as well as energy consumption optimisation, predictive maintenance, predict process behaviour, supply chain, remote operation.

Non-ferrous metals: ML approaches are suggested by [30] for inspecting aluminum structure subjected to temperature changes and by [31] to address the identification of the atoms in the grain boundary regions of the aluminum. In [32], the orthogonal test method and DV are used to observe the effect of multifactor composite action on copper slag to reduce serious environmental problems. ESs are proposed for the analysis of aluminum electrolysis an ES is proposed in [33] for monitoring and emergency decisions of the tank condition of the electrolytic aluminum and for automated inspection system of the spraying parameters splats [34].

Water sector: it is showed a significant application of digital technologies in the sector. ML is applied in the SC (re)configuring and scheduling and R&D activities for different purposes ranging from energy and resource efficiency in the water distribution systems [35], cost reduction of raw material in water treatment plants, and decision support systems based on artificial neural network application in water and wastewater [36]. IP and IA pursue the sustainability and efficiency in multi-sectoral water allocation [37], the optimization of water infrastructure resilience and performance [38], and the smart utilisation of wastewater storage capacity to prevent flooding. Finally, OSR technologies (e.g. GIS-integrated simulation models) have been developed for the conjunctive use of surface and groundwater and water-constrained agricultural production. As for BD, data collection and BD analytics are applied to monitor water pipeline infrastructure systems [39], DV for wastewater contaminants understanding [40] and DM techniques for hydro informatics purposes [41].

Chemicals: digital transformation driving major opportunities [42] in the sector. ML application based on artificial neural networks (e.g. neuro-fuzzy) within different control loops are applied for network predictive control regarding energy savings [43]. Most of the studies focused on technologies related to DUC, and ML to predict higher heating values of a biomass [44] and energy use and GHG emissions reduction [45]. BD (mainly DM and DC and SI) are applied for data interoperability supporting computational toxicology and chemical safety evaluation [46] and CSI technologies in development activities of the chemical industry [47,48].

Table 1 shows the “heat map” of the references found in the literature search. It can be seen that the “hot” technology category is ML with major applications to the chemical and minerals sectors. It is notable that there are still several areas to be investigated and were the application to the analysed sectors are still limited. DUC, DPR and CSI are still to be investigated with specific focus on these sectors of the process industry, most probably, this is due to the fact that these categories are complementary to other technologies and a transversal approach, sector independent, has been applied till now.

Process industry sectors	DUC	NLP	OSR	ML	IP	ES	CBR	IA	CPS	DV	DP	DPR	DM	CSI
Cement				4		3	1		1	2	2		1	
Ceramics			2	4	4	2	1	1	2	1	4		2	
Chemicals	8		1	10			1		1		2		3	3
Engineering	1	8		5	1	4	4	4	8	1		1	5	3
Minerals	2	1	4	14	4	1	1	2	1	1	1	1	3	2
Non ferrous metals				7		2	1		1	1	3		1	
Steel		2	5	8		7	1	2	5		2		2	
Water		1	1	7	1			1	1	2	2		3	

HEAT MAP
> 9 high
4-9 medium
0-3 low

Fig. 1. Heat map of AI/BD for process industry

4 CONCLUSIONS

Based on the LR presented shortly in the previous sections, the findings of the paper can be used as a guideline for defining the areas along which to further investigate and where there is a gap to define development paths in the future. In particular:

- *Market analysis and open innovation*: need for forecasting based on intelligent system for customer relationships management and online monitoring and order management systems for the suppliers. Improvements in this area is necessary both for sectors dealing with final consumer (i.e. ceramic) as well as for B2B sectors (i.e. chemical, steel, …) that are "far" from the final market but need to forecast demand of final products to make production planning.
- *Process control and optimisation*: companies in Process Industry need to have support for the real-time integrated control of the different production phases enabling CPS by new way to formalize and treat BD collected along the process from machines, devices etc. to avoid workers to dangerous working conditions. In these sectors with continuous flow of material, it is important to find a way to assure raw material quality control by automatic visual classification and advanced sensing systems with a high precision and timely manner. For what concerns monitoring of inventory level, some areas are related to positioning of the raw material and resources (e.g. internal transport modes) in the warehouse, operators' guide for timely picking and loading activities.
- *Predictive maintenance:* this area is already covered in many sectors but there is the need to further investigate for the development of algorithms based on different types of AI like neural-networks, deep learning etc taking into account the specificity of the production equipment used in each sector.
- *Research and innovation:* it is necessary to further develop AI/BD technologies supporting management, planning and design of research and innovation. Innovation at product level can be supported by AI/BD for designing, simulating, testing product features. Tools for automatic alignment in the design of product and process is also important. Dealing with the sustainability of the new generation of products is also

an important issue and all the data collected with DUC, DP and DM can enable evaluation of energy efficiency and environmental impact.
- *Supply chain:* this area includes all the operational perspectives related to configuration, planning and management of SC. Some important ongoing trends related to Process Industry need to be taken into consideration like industrial symbiosis and value chain integration for circular economy: AI/BD can facilitate the forward flows of the raw materials and primary products, but also manage and integrate it with the reverse flows to the factory, waste management systems, and other value-added activities.

A cross-cutting area of analysis is related to the ethical and social dimension arisen by AI/BD techniques incorporating hybridization of intelligent systems with humans and the role of the AI/BD systems combined with other methods and tools in pandemic situations such as COVID-19 should be studied to define paths to provide new production models to avoid risk propagation.

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References

1. Ransbotham, S., Kiron, D., Gerbert, P., and Reeves, R.: Reshaping Business with Artificial Intelligence. In: MIT Sloan Management Review and The Boston Consulting Group (2017).
2. Wuest, T., Weimer, D., Irgens, C. and Thoben, K.-D.: Machine learning in manufacturing: advantages, challenges, and applications. Production & Manufacturing Research 4(1), pp. 23–45 (2016).
3. Wang, Y., Li, X., Tsung, F.: Configuration-Based Smart Customization Service: A Multitask Learning Approach. IEEE Transactions on Automation Science and Engineering 17(4), pp. 2038-2047 (2020).
4. AI-Cube Homepage, https://www.ai-cube.eu/, last accessed 2021/07/08.
5. Samoili, S., Lopez Cobo, M., Gomez Gutierrez, E., De Prato, G., Martinez-Plumed, F., Delipetrev, B.: AI WATCH. Defining Artificial Intelligence. Publications Office of the European Union, Luxembourg (2020).
6. Zhang, M., Sun, C. N., Zhang, X., Wei, J., Hardacre, D., & Li, H.: Predictive models for fatigue property of laser powder bed fusion stainless steel 316L. Materials & Design 145, 42-54 (2018).
7. Ruiz, E., Ferreño, D., Cuartas, M., López, A., Arroyo, V., Gutiérrez-Solana, F.: Machine learning algorithms for the prediction of the strength of steel rods: an example of data-driven manufacturing in steelmaking. International Journal of Computer Integrated Manufacturing 33(9), 880-894 (2020).
8. Karagiorgou, S., Vafeiadis, G., Ntalaperas, D., Lykousas, N., Vergeti, D., Alexandrou, D.: Unveiling Trends and Predictions in Digital Factories. In 15th International Conference on Distributed Computing in Sensor Systems (DCOSS) 2019, pp. 326-332 (2019).

9. Kong, Y., Chen, D., Liu, Q., Long, M.: A prediction model for internal cracks during slab continuous casting. Metals 9(5), pp. 587-604 (2019).
10. Klinger A., Altendorfer A., Bettinger D., Hughes G.D., Al-Husseini A.A., Gupta D.R.: The new system for control and improvement of technological process at DRI units. Chernye Metally 10 (2017).
11. Kang, L. W., Chen, Y. T., Jhong, W. C., & Hsu, C. Y.: Deep learning-based identification of steel products. In: International Conference on Intelligent Information Hiding and Multimedia Signal Processing, pp. 315-323. Springer, Cham (2018).
12. Fumagalli, L., Cattaneo, L., Roda, I., Macchi, M., & Rondi, M. Data-driven CBM tool for risk-informed decision-making in an electric arc furnace. The International Journal of Advanced Manufacturing Technology, 105(1-4), 595-608 (2019).
13. Wichmann, P., Brintrup, A., Baker, S., Woodall, P., McFarlane, D.: Extracting supply chain maps from news articles using deep neural networks. International Journal of Production Research 58(17), pp. 5320-5336 (2020).
14. Park, J., Ferguson, M., Law, K. H.: Data Driven Analytics (Machine Learning) for System Characterization, Diagnostics and Control Optimization. In: Smith I., Domer B. (eds) Advanced Computing Strategies for Engineering, LNCS, vol. 10863. Springer, Cham. (2018).
15. Herrera, M., Pérez-Hernández, M., Parlikad, A. K., & Izquierdo, J.: Multi-agent systems and complex networks: Review and applications in systems engineering. Processes 8(3), pp. 312-341 (2020).
16. Shcherbakov M.V., Glotov A.V., Cheremisinov S.V.: Proactive and predictive maintenance of cyber-physical systems. In: Cyber-Physical Systems: Advances in Design & Modelling, pp. 263-278. Springer, Cham. (2020).
17. Cheng, D., Zhang, J., Hu, Z., Xu, S., & Fang, X.: A digital twin-driven approach for on-line controlling quality of marine diesel engine critical parts. International Journal of Precision Engineering and Manufacturing 21(10), 1821–1841 (2020).
18. Colombo, E. F., Shougarian, N., Sinha, K., Cascini, G., & de Weck, O. L.: Value analysis for customizable modular product platforms: Theory and case study. Research in Engineering Design 31(1), 123–140 (2020).
19. Tripathi, G., Anowarul, H., Agarwal, K., Prasad, D.K.: Classification of Micro-Damage in Piezoelectric Ceramics Using Machine Learning of Ultrasound Signals. Sensors 19(19), 4216 (2019).
20. Nakai, M.E., Aguiar P.R., Guillardi, H., Bianchi, E.C., Spatti D.H., D'Addona, D.M.: Evaluation of neural models applied to the estimation of tool wear in the grinding of advanced ceramics. Expert Systems with Applications 42(20), 7026-7035 (2015).
21. Qian, Z., QingLong, M., YongQian, X., Gan Lin, G.: The Robot Intelligent Spraying Glazing System for Sanitary Ceramics Industry. J. Phys.: Conf. Ser. 1653 012028 (2020).
22. Ghayour, H., Abdellahi, M., Bahmanpour, M.: Artificial intelligence and ceramic tools: Experimental study, modeling and optimizing. Ceramics International 41(10) Part A, 13470-13479 (2015).
23. Sadegh Amalnik, M.: Expert System Approach for Optimization of Design and Manufacturing Process for Rotary Ultrasonic Machining. ADMT Journal, 11(1), pp. 1-13 (2018).
24. Shi. Y., Zhang, Y., Baek, S., De Backer, W., Harik, R.: Manufacturability analysis for additive manufacturing using a novel feature recognition technique. Computer-Aided Design and Applications 15(6), 941-952 (2018).
25. Braccini, A.M., Margherita, E.G.: Exploring Organizational Sustainability of Industry 4.0 under the Triple Bottom Line: The Case of a Manufacturing Company. Sustainability 11(1), 36 (2019).

26. Faisal, Md., Katiyar, V.: Identification of essential requirements of IOT and big data analytics to extend ceramic manufacturing. International Journal of Engineering Sciences & Research Technology (IJESRT) 5(12), 919- 923 (2016).
27. Key Stages in the Mining Process, https://www.cornwall.gov.uk/environment-and-planning/conservation/world-heritage-site/delving-deeper/mining-processes/key-stages-in-the-mining-process/, last accessed 2021/07/08.
28. Trends in Modern Mining Technology. https://www.angloamerican.com/futuresmart/stories/our-industry/technology/trends-in-modern-mining-technology
29. AI Powering the future of cement, Cement World. May 2020. https://www.worldcement.com/special-reports/11052020/ai-powering-the-future-of-cement/, last accessed 2021/07/08.
30. Vitola, J., Pozo, F., Tibaduiza, D. A., & Anaya, M.: Distributed piezoelectric sensor system for damage identification in structures subjected to temperature changes. Sensors, 17(6), 1252 (2017).
31. Gomberg, J. A., Medford, A. J., & Kalidindi, S. R.: Extracting knowledge from molecular mechanics simulations of grain boundaries using machine learning. Acta Materialia 133, 100-108 (2017).
32. Lan, W., Wu, A., Yu, P.: Development of a new controlled low strength filling material from the activation of copper slag: Influencing factors and mechanism analysis. Journal of Cleaner Production 246 (2020).
33. Li, L., Xie, Y., Chen, X., Yue, W., & Zeng, Z.: Dynamic uncertain causality graph based on cloud model theory for knowledge representation and reasoning. International Journal of Machine Learning and Cybernetics, 1-19 (2020).
34. Mulero, M. A., Zapata, J., Vilar, R., Martínez, V., Gadow, R.: Automated image inspection system to quantify thermal spray splat morphology. Surface and Coatings Technology 278, 1-11, (2015).
35. Bagloee, S. A., Asadi, M., & Patriksson, M.: Minimization of water pumps' electricity usage: A hybrid approach of regression models with optimization. Expert Systems with Applications 107, 222-242 (2018).
36. Hadjimichael, A., Comas, J., & Corominas, L.: Do machine learning methods used in data mining enhance the potential of decision support systems? A review for the urban water sector. AI Communications, 29(6), 747-756 (2016).
37. Zhou, Y., Chang, L. C., Uen, T. S., Guo, S., Xu, C. Y., & Chang, F. J.: Prospect for small-hydropower installation settled upon optimal water allocation: An action to stimulate synergies of water-food-energy nexus. Applied Energy 238, 668-682 (2019).
38. Facchini, A., Scala, A., Lattanzi, N., Caldarelli, G., Liberatore, G., Dal Maso, L., & Di Nardo, A.: Complexity science for sustainable smart water grids. In Italian Workshop on Artificial Life and Evolutionary Computation, pp. 26-41. Springer, Cham (2016).
39. Sinha, S., Sears, L.: Collection and Compilation of Water Pipeline Field Performance Data. In: Pipelines 2017, pp. 124-135 (2017).
40. Ponce Romero, J. M., Hallett, S. H., Jude, S.: Leveraging big data tools and technologies: addressing the challenges of the water quality sector. Sustainability, 9(12), 2160 (2017).
41. Chen, Y., Han, D.: Big data and hydroinformatics. Journal of Hydroinformatics 18(4), 599-614 (2016).
42. Piccione, P. M.: Realistic interplays between data science and chemical engineering in the first quarter of the 21st century: Facts and a vision. Chemical Engineering Research and Design 147, 668-675 (2019).

43. Kramer, A., Morgado-Dias, F.: Artificial intelligence in process control applications and energy saving: a review and outlook. Greenhouse Gases: Science and Technology 10(6), 1133-1150 (2020)
44. Ighalo, J. O., Adeniyi, A. G., Marques, G.: Application of linear regression algorithm and stochastic gradient descent in a machine-learning environment for predicting biomass higher heating value. Biofuels, Bioproducts and Biorefining 14(6), 1286-1295 (2020).
45. Makarova, A. S., Jia, X., Kruchina, E. B., Kudryavtseva, E. I., Kukushkin, I. G.: Environmental performance assessment of the chemical industries involved in the Responsible Care® Program: Case study of the Russian Federation. Journal of Cleaner Production 222, 971-985 (2019).
46. Watford, S., Edwards, S., Angrish, M., Judson, R. S., Friedman, K. P.: Progress in data interoperability to support computational toxicology and chemical safety evaluation. Toxicology and applied pharmacology 380 (2019).
47. McDonagh, J. L., Swope, W. C., Anderson, R. L., Johnson, M. A., Bray, D. J.: What can digitisation do for formulated product innovation and development? Polymer International 70(3), 248-255 (2020).
48. Pellis, A., Cantone, S., Ebert, C., Gardossi, L.: Evolving biocatalysis to meet bioeconomy challenges and opportunities. New biotechnology 40, 154-169 (2018).