WNIOSEK
O WSZĘCIE POSTĘPOWANIA HABILITACYJNEGO

Załącznik 2b
AUTOREFERAT W JĘZYKU ANGIELSKIM

Dr inż. Joanna Guziałowska-Tic

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Annex 2b

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SUMMARY OF PROFESSIONAL ACCOMPLISHMENTS

1. Name and surname

Joanna Guziałowska-Tic

Previous surname: Guziałowska

2. Diplomas

2004 **Master's degree in environmental engineering**

Opole University of Technology, Faculty of Mechanical Engineering

Master's thesis: „The study of heat flow irregularity in the tube space of the exchanger". Supervisor: prof. dr hab. inż. Roman Ulbrich.

2008 **Doctoral degree, doctor of technical sciences in the field of mechanical engineering**

Opole University of Technology, Faculty of Mechanical Engineering

Doctoral thesis: „The study of two phase gas-liquid flow in the exchanger with baffles". Supervisor: prof. dr hab. inż. Roman Ulbrich, reviewers: prof. dr hab. inż. Stanisław Witczak, prof. dr hab. inż. Teodor Skiepko.

2011 **Postgraduate studies in Chemistry and environmental chemistry**

University of Wroclaw, Faculty of chemistry

3. Information on previous employment in scientific units

2008–2010 **Assistant** in Department of Environmental Engineering, Faculty of Mechanical Engineering, Opole University of Technology.

2010–present **Adjunct** in Department of Environmental Engineering, Faculty of Mechanical Engineering, Opole University of Technology.

4. Indication of scientific achievement

4.1. Title of scientific achievement

As a scientific achievement, resulting from art. 16 sec. 2 of the Act of 14 March 2003 on academic degrees and the academic title as well as on degrees and title in the field of art (Journal of Laws No. 65, item 595 with later amendments), I indicate a series of eleven related publications entitled: **„ Assessment of the impact of environmentally friendly products on the environment using experimental research and quantitative relationship between chemical structure and biological activity (QSAR)".**

4.2. Publications cycle

The achievement indicated for the assessment in the habilitation procedure is the cycle of eleven articles published in 2009-2018 regarding the impact of environmentally friendly products on the environment using different methods:

ON1. Wilhelm Jan Tic, **Joanna Guziałowska**, 2009, Nowoczesne rozpuszczalniki i koalescenty farb i lakierów w świetle wymagań REACH, Środowisko i Rozwój, 20, 55-70. MNiSW (2009): **2 points.**

ON2. Wilhelm Jan Tic, **Joanna Guziałowska-Tic**, 2011, Badania nad technologią wytwarzania katalizatorów ekologicznego spalania ciężkich olejów opałowych, Zeszyty

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Naukowe Politechniki Rzeszowskiej nr 276, Budownictwo i Inżynieria Środowiska, 58 (4/11), 301-308. MNiSW (2011): **4 points.**

ON3. Joanna Guziałowska-Tic, Wilhelm Jan Tic, 2012, Enviromentally-friendly solvents for paints and varnishes in the light of REACH – synthesis, toxicological and ecotoxicological properties, Polish Journal of Environmental Studies, 21(5A), 419-424.

ON4. Joanna Guziałowska-Tic, Wilhelm Jan Tic, 2015, Toxicological and ecotoxicological properties of an iron based combustion modifier for liquid fuels, Ecological chemistry and engineering A, 22(2), 161-173. MNiSW (2015): **11 points.**

ON5. Joanna Guziałowska-Tic, Wilhelm Jan Tic, 2015, Wpływ żelazowego modyfikatora spalania paliw ciekłych na środowisko glebowe, Przemysł Chemiczny, 94(9), 1518-1520. IF (2017): **0,367**; MNiSW (2015): **15 points**.

ON6. Joanna Guziałowska-Tic, Wilhelm Jan Tic, 2016, Study on the Biodegradability of Organometallic Modifier Used in Liquid Fuel Combustion, Polish Journal of Environmental Studies, 25(4), 1515 – 1522. IF (2016): **0,793**; MNiSW (2016): **15 points**.

ON7. Joanna Guziałowska-Tic, 2017, The use of QSAR methods for determination of n-octanol/water partition coefficient using the example of hydroxyester HE-1, E3S Web of Conferences, 19, 02034. MNiSW (2017): **15 points**.

ON8. Joanna Guziałowska-Tic, 2017, The use of QSAR methods to determine physicochemical properties on the example of 3-hydroxy-2,2,4-trimethylpentylisobutyrate, Przemysł Chemiczny, 96(8), 1673-1676. IF (2017): **0,399**; MNiSW (2017): **15 points**.

ON9. Joanna Guziałowska-Tic, Wilhelm Jan Tic, 2017, Effect of an iron based modifier for liquid fuels combustion on the aquatic environment, Journal of Cleaner Production, 165, 1197-1203. I IF (2017): **5,651**; MNiSW (2017): **40 points**.

ON10. Joanna Guziałowska-Tic, Wilhelm Jan Tic, 2018, Analysis of the adverse impact of an iron-based combustion modifier for liquid fuels on human health, Journal of Cleaner Production, 174, 1527-1533. IF (2017): **5,651**; MNiSW (2017): **40 points**.

ON11. Joanna Guziałowska-Tic, 2018, Assessment of the impact of an iron-based modifier for heating oil combustion on the environment using the Vega in silico tool, Przemysł Chemiczny, 97(9), 1474-1476. IF (2017): **0,399**; MNiSW (2017): **15 points**.

The above-mentioned publications constitute a monothematic cycle, were prepared for a predetermined subject and were published cyclically in 2009-2018. As it was shown in the rest of the Self-review, the research described in the publications was planned as a multi-stage research program. The contribution of co-authors in the publications listed as a scientific achievement was presented in the statements in Annex 4 to the application.

4.3. Discussing of the scientific goal

4.3.1. Introduction

Human industrial activities often have a negative impact on the natural environment. It is not always possible to maintain the balance between new technologies and the protection of natural resources. The rapid development of technology and changes that take place in the modern world have a significant impact on the natural environment. It is required that industrial development should be sustainable and does not cause degradation of the natural environment, while at the same time enabling the needs of present and future generations to be met (Tic, 2016).

An important aspect introduced in industrial activities are environmentally friendly solutions favoring the maintenance of balance in nature. These solutions are closely related to the projects undertaken by the industries in the field of environmental engineering. Often such solutions are additives/modifiers, which are added, for example, to fuels to reduce the emission of harmful substances into the atmosphere, or new products – chemical substances that are safe for the environment.

In connection with the coming into the force of the REACH Regulation, manufacturers and importers of chemical substances with a tonnage of more than 1 Mg/year are required to prepare a chemical safety assessment as a part of product registration. Such a document aims to determine the impact of a given chemical substance on the environment and human health. In order to prepare a chemical safety assessment of the product, it is necessary to perform physicochemical, toxicological, ecotoxicological and environmental tests (REACH, 2006). Unfortunately, some of these studies, especially for substances manufactured or imported in high tonnage (above 100 Mg/year), are carried out on experimental animals. In the case of the assessment of harmful properties, the most frequently used are experimental animals (rats and mice), but also rabbits, guinea pigs, fish, and in rare cases also birds (ECHA, 2012).

The chemical safety assessment of products for the purpose of their registration requires tests to determine their physicochemical, toxicological and ecotoxicological properties. Unfortunately, some of those tests involve the use of animals. After the coming into force of the Directive of the European Parliament and of the Council No. 2010/63/EU of 22 September 2010 concerning the protection of animals used for scientific purposes, the number of experiments involving the use of animals has to be reduced so as to ease their pain and suffering in connection with the tests (Directive, 2010). According to the provisions of the Directive, the target is to eliminate the unnecessary tests on animals. REACH requires that the registrants should restrict new tests with the use of vertebrates for the purpose of registration and use them only as a last resort (Lilienblum et al., 2008). First, it is necessary to collect and assess all existing data concerning the test substance and then, to detect any data gaps and consider the possibility of filling them with the results of in vitro/ex vivo tests or other, alternative concepts (Fig. 1). Another option is to use information based on tests involving human exposure, predictions based on available information about substances with similar structures (e.g., "cross-sectional approach" or "chemical categories"), as well as expectations based on reliable quantitative prediction methods, such as quantitative structure-activity relationships (QSAR) (Patel et al., 2014).

In many literature reports, the authors describe the use of QSAR methods to assess the impact of chemical substances on the environment and human health. These are theoretical models for the qualitative or quantitative prediction of physicochemical, biological properties and the fate of the compound in the environment based on the knowledge of their chemical

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structure. In order to determine the properties of the chemical, the reliability of the QSAR model and verification if the test substance is in the field of application of the model should be assess, in order to obtain a reliable estimate. A very important element in QSAR modeling is well identified structure of a chemical substance. In the case of multi-constituent substance it is needed to identify all of its components, as well as take into account all impurities and additives. If there are stable reaction products of a substance, it should be also identified. As a rule, it is required to present the appropriate structure of the chemical and if necessity the stereochemistry should also be considered.

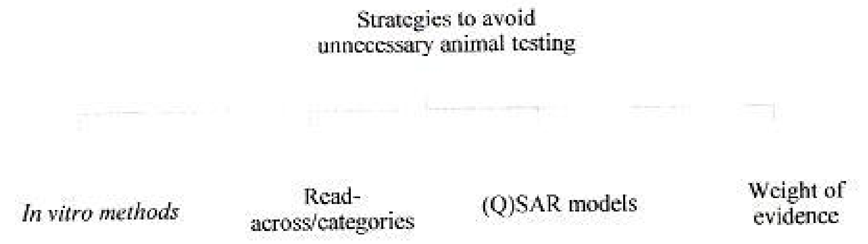

Figure 1. Strategies to avoid unnecessary animal testing (Guziałowska-Tic, 2016)

From year to year we can observe an increasing interest in QSAR methods used to determine toxicological and ecotoxicological properties as part of product registration. According to recent data from the European Chemicals Agency, of the 6,290 analyzed substances, for endpoints on tests on vertebrates, almost 34% of substances contain at least one information on the tested properties using the QSAR method (ECHA, 2017).

In order to facilitate access to QSAR methods, there are many publicly available software to determine physicochemical, toxicological, ecotoxicological and environmental properties. Tables 1 and 2 present the available software used to assess the physicochemical, toxicological, ecotoxicological and environmental properties which, according to the REACH Regulation and depending on the tonnage of the substance being manufactured or imported, are necessary to be tested in order to registration of the product (ANTARES, 2011).

In addition to the commonly available software presented in Tables 1 and 2, the European Chemicals Agency also provides the OECD QSAR Toolbox on its website. This tool can be used to complete the toxicity and ecotoxicity data that are needed at the stage of risk assessment related to the use of chemical substances (Dimitrov et al., 2016).

Mays et al., presented the results of a questionnaire which was conducted among the academic staff, officials and company employees and which concerned benefits and barriers in using QSAR under REACH. The responders indicated that their preferred QSAR methods were OECD Toolbox, EPISuite and CAESAR. It was then observed that, in the case of physicochemical properties, the QSAR methods were primarily used for determination of the partition coefficient. In the case of toxicological properties, QSAR methods were primarily used for determination of mutagenicity, cancerogenicity and teratogenicity; in the case of environmental fate, the QSAR methods were primarily used for determination of acute toxicity to daphnia and toxicity to fish. In ecotoxicological test, numerical methods were mainly used for determination of bioaccumulation and biodegradability – though only by scientists and officials (Mays et al., 2012).

Table 1. Review of available software enabling determination of the physicochemical and toxicological properties of substances without experimental methods, acc. to (ANTARES, 2011)

Property tested	Software
Physico-chemical properties	
Melting/freezing point	EPI Suite
Boiling point	Epi Suite, SPARC, T.E.S.T.
Relative density	T.E.S.T.
Vapour pressure	Epi Suite, SPARC
Surface tension	T.E.S.T.
Water solubility	EPI Suite, OSIRIS, SPARC, T.E.S.T., VCCLAB
Melting/freezing point	EPI Suite
Boiling point	Epi Suite, SPARC, T.E.S.T.
Relative density	T.E.S.T.
Vapour pressure	Epi Suite, SPARC
Toxicological properties	
Skin irritation or skin corrosion	ToxTree, BfR-DSS
Eye irritation	ToxTree, BfR-DSS
Skin sensitization	VEGA, CAESAR
In-vitro gene mutation study in bacteria	VEGA, CAESAR, OSIRIS, Lazar, ToxTree, T.E.S.T.
In-vitro citogenicity study in mammalian cells or in-vitro micronucleus study	ToxPredict
In-vivo mutagenicity study	ToxTree
Acute toxicity (by oral route)	T.E.S.T.
Acute toxicity (by inhalation)	none found
Repeated dose toxicity (28 days)	Lazar
Reproductive toxicity	IST, VEGA, OSIRIS, CAESAR
Assessment of toxicokinetic behavior of the substance	ToxPredict, Althotas Virtual Laboratory, IndusChemFate, PBPK/MEGen

There are many reports in the literature describing the use of QSAR methods to determine the bioconcentration factor, genotoxicity, as well as toxicity to fish and daphnia. Petoumenou et al. (2015) and Gissi et al (2015) used the VEGA and T.E.S.T platforms to determine the bioconcentration factor (BCF). Wedebye et al. (2015), using the QSAR methods, examined nearly 71,000 substances for the assessment of carcinogenic genotoxicity, mutagenicity and developmental toxicity. The results of studies on the impact of toxicity of chemical substances on Daphnia and fish, using the quantitative dependence between chemical structure and biological activity, have been described in Cassani et al (2013), Petrescu et al (2015), Cappelli et al (2015), Golbamaki and others (2014).

Table 2. Review of available software enabling determination of the ecotoxicological and environmental properties of substances without experimental methods, acc. to (ANTARES, 2011)

Ecotoxicological properties	
Short-term toxicity testing on invertebrates (daphnia)	Demetra, EPI Suite, T.E.S.T.
Growth inhibition study aquatic plant (algae preferred)	EPI Suite
Short-term toxicity testing on fish	ToxPredict, VEGA, Demetra, EPI Suite, Lazar, T.E.S.T.
Activated sludge respiration inhibition testing	EPI Suite
Long-term toxicity testing invertebrates (preferred daphnia)	EPI Suite
Long-term toxicity testing on fish	EPI Suite
Short-term toxicity to invertebrates	EPI Suite, Demetra
Short-term toxicity to plants	EPI Suite
Environmental properties	
Ready biodegradability	EPI Suite, ToxPredict, VEGA, CRAFT
Soil simulation testing	EPI Suite
Abiotic dagradation	EPI Suite
Hydrolysis as a function of pH	EPI Suite, SPARC
Identification of degradation products	BiotS, UM-BBD Pathway Prediction System, CRAFT
Absorption/desorption screening	EPI Suite, BASL4
Bioaccumulation in aquatic species, preferable fish	VEGA, EPI Suite, CAESAR, Fish Model, TAOBAC model, T.E.S.T.
Further information on the environmental fate and behavior of the substance	EPI Suite

The analysis of literature reports indicates, that the compatibility between the results of experimental research and those from QSAR methods is not always satisfactory. This compliance depends primarily on the correctly selected model and descriptor.

4.3.2. Scientific goal

Despite the growing popularity of the QSAR methods to determine the impact of chemical substances on the environment and human health, however publications describing groups of compounds of similar structure dominate, for which only single physicochemical, toxicological, ecological and environmental properties are analyzed. The results from QSAR methods are still used as support in grouping substances, cross-sectional approaches and in the weight of evidence, as well as supplementing information on the substance. Among other things

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from the work of Wedebye et al. (2015) it follows that QSAR methods in the case of genotoxic carcinogenicity, mutagenicity and developmental toxicity can be used only in combination with the results of experimental studies (on animals) and other information available in the literature. Low interest in QSAR methods is related to the fact that these methods give the best results in the case of compounds with simple structures, whereas in the case of multicomponent substances and those that contain a lot of impurities, these methods are not fully effective.

Therefore, the basic **scientific goal** of the publication cycle, which is a scientific achievement indicated for the assessment in the habilitation procedure, is the assessment of the applicability of methods of quantitative dependence between chemical structure and biological activity, on the example of two selected products:

a) 3-hydroxy-2,2,4-trimethylpentyl isobutyrate (Hydroxyester HE-1) - an environmentally-friendly additive for paints and varnishes,

b) iron-based combustion modifier for liquid fuels - as an example of a multicomponent substance, which is a mixture of four ingredients.

For the accomplishment of the scientific goal described above, many-year studies have been carried out, which can be divided into three stages:

1. Synthesis of Hydroxyester HE-1 [ON1, ON3] and iron-based combustion modifier for liquid fuels [ON2] and evaluation of their innovativeness and environmentally friendly in relation to products present on the market.
2. Execution and analysis of physicochemical, toxicological, ecotoxicological and environmental tests results for the Hydroxyester HE-1 [ON1, ON3, ON8] and iron-based combustion modifier for liquid fuels [ON4, ON5, ON6, ON9, ON10] to determine their impact on the environment and human health.
3. Assessment of the possibility of using QSAR methods to determine the effect of Hydroxyester HE-1 [ON7, ON8] and iron-based combustion modifier for liquid fuels on the environment and human health [ON11] to replace animal testing.

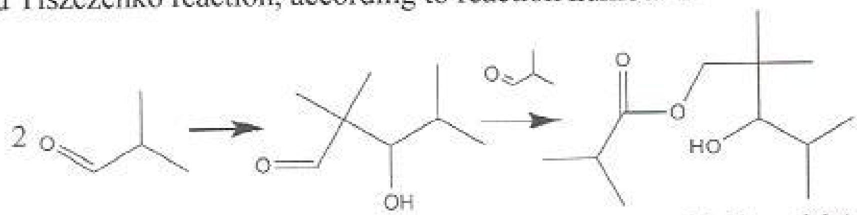
4.4. Discussion of research results

4.4.1. Synthesis of environmentally friendly products

Hydroxyester HE-1

The Hydroxyester HE-1 is obtained in a sequence of chemical reactions: aldol condensation process with isobutyric aldehyde as the basic material, followed by the Cannizaro and Tiszczenko reaction, according to reaction number 1:

(1)



isobutyl aldehyde 3-hydroxy-2,2,4-trimethylpentanal 3-hydroxy-2,2,4-trimethylpentyl isobutyrate (Hydroxyester HE-1)

Hydroxyester HE-1 is a hydrophobic organic solvent whose main direction of use is the coalescent function in water-soluble architectural paint formulations and is an alternative to toxic solvents and coalescents used in the production of paints and varnishes [ON1, ON3].

The boiling point was determined for this product according to OECD guideline No. 103 and was 255 ° C. Depending on the formal definitions and methods of evaluation criteria, Hydroxyester HE-1 in various regions of the world is subject to different qualification as volatile organic compound (VOC). In accordance with the European Union Directive 2004/42 / EC, which accepts the boiling point above 250 ° C as the criterion of VOC classification, Hydroxyester HE-1 is not included in the group of volatile organic compounds. On the Chinese market HE-1 is qualified as a safe and eco-friendly product. In the United States, according to EPA, method 24, Hydroxyester HE-1 is considered 100% volatile Organic Compound (Sparks et al., 1999, Chang et al., 1999).

As the part of research in the NCBR project entitled: "Commercialization of the production technology of isobutyl aldehyde trimer as a substitute for aromatic derivatives for the production of modern solvents and surfactants", the concept of launching the production of safe solvents and coalescents was established, based on the possibility of managing the existing raw materials and technical facilities of the Oxo installation in Azoty Group in Zakłady Azotowe Kędzierzyn SA (Annex 3, point II.J.1). In the face of restrictions on the use of toxic phthalate solvents, production of the Hydroxyester HE-1 in the amount of 100 to 1000 Mg/year is planned.

The obtained product is protected by a Polish patent claiming the composition of the reaction mixture (Annex 3, point II.C.3) and the European patent claiming the condensation parameters of isobutyraldehyde to the Hydroxyester HE-1 and the method of separating the product with high purity (Annex 3, point II.C. 2), which I am a co-author (Annex 3 point II.C). In the patent (Annex 3, point II.C.1), a method of synthesis of a latex composition for the manufacture of waterborne paints and varnishes was claimed, in which a modern, environmentally safe coalescing - Hydroxyester HE-1 was applied. Innovative manufacturing technology of Hydroxyester HE-1was awarded at national and international exhibitions of inventions (Annex III, point III.D.2-5).

Iron-based combustion modifier for liquid fuels

In the synthesis process were used: hydrated iron (III) sulphate, fatty acids, NH_3 solution (25%) and diesel oil. The synthesis of the modifier was proceeded in two stages, according to reactions (2) and (3):

$$Fe_2(SO_4)_3 + 6NH_3 + H_2O \rightarrow 2Fe(OH)_3 + 3(NH_4)_2SO_4 \qquad (2)$$

$$Fe(OH)_3 + 3R\text{-}COOH \rightarrow (R\text{-}COO)_3Fe + 3H_2O \qquad (3)$$

In first stage, ammonia water was added to the solution obtained by dissolving the metal salt in water. A solution prepared by dissolving fatty acids in diesel oil was added to the solution prepared in this way. After the reaction, the organic phase was separated from the aqueous one.

The organic phase was an iron additive containing 200g Fe/dm^3 of solution. The obtained products are highly soluble in the tested fuel and are not stratified [ON2].

The next stage of the research was the evaluation of the catalytic efficiency of the iron modifier in the mazut combustion tests in the measurement system for fuel calorimetry. The test apparatus was equipped with a Junkers flow calorimeter and a liquid fuel flow and exhaust gas flow measurement system. The applied system allowed to determine the thermal balance of the fuel combustion process in the presence of the modifier and without, and the mass balance of the combustion process. In the fuel tests without an additive, and with the addition of Fe was used. The parameters of fuel combustion tests (mazut) were as follows: metal concentration in the fuel burned was 60 ppm, the mazut flow rate was 1200 cm^3/h, and the excess of air was 2. The research confirmed the beneficial effect of the modifier on the combustion process. In combustion tests, an additional heat gain was obtained by 8% and NO_x emission reduction by 9% [ON2].

The obtained test results were verified on a pilot scale in the combustion tests in a 400 KW boiler. During the tests, the amount of ash produced was reduced, the SO_2 emissions were reduced by 7%, NO_x by 3% and the efficiency of the boiler increased by 4%. During the combustion tests, a reduction in the amount of sediments formed on the grate and in the combustion chamber was also observed. The obtained test results confirmed the beneficial effect of the iron modifier on the combustion process of the mazut [ON2].

The research was carried out as part of the project: "Research on the energy-ecological efficiency system for the combustion of liquid and solid fuels" (Annex 3, point II.J.3), of which I was the contractor. It is planned to launch the production of iron-based combustion modifier for liquid fuels in quantities from 100 to 1000 Mg/year.

The technology for producing the iron-based modifier was awarded at the international exhibition of inventions (Annex 3, point III.D.1).

4.4.2. Execution and analysis of physicochemical, toxicological, ecotoxicological and environmental tests results

Due to the fact that production of the Hydroxyester HE-1 and the iron-based combustion modifier for liquid fuels are planned in the quantity from 100 to 1000 Mg, according to the REACH regulation, it was necessary to perform a chemical safety assessment of these products. Therefore, for the discussed products, physicochemical, toxicological, ecotoxicological and environmental tests were performed. Because in accordance of REACH requirements, such tests must be carried out in accordance with good laboratory practice in certified laboratories, the above tests have been commissioned to a specialized unit. Toxicological, ecotoxicological and environmental studies were carried out at the Institute of Organic Industry in Warsaw, a branch in Pszczyna, and physicochemical research at the Institute of Heavy Organic Synthesis "Blachownia". These studies were commissioned as part of two projects at the Opole University of Technology and West Technology & Trading Polska (Annex 3, point II.J.1 and section II.J.3), in which I was one of the main contractors and personally was responsible for this part of research. I chose the schedule necessary to perform the tests based on the assumed production volume and requirements contained in the REACH regulation.

Hydroxyester HE-1

In the case of physicochemical tests, eight properties were made according to the REACH guidelines for the assumed production scale. All tests were performed in accordance with the OECD guidelines and European Community regulations. Table 3 summarizes the obtained results.

Based on the test results, it was found that the boiling temperature was 255 ° C, which confirms that Hydroxyester HE-1 is not classified as a volatile organic compound and can be safely used as coalescent in paint and varnish formulations. In turn, the partition coefficient n-octanol/water (log P) was 2.1. Log P (log Kow) is an important parameter in the chemical safety assessment of a substance, CLP classification and PBT assessment. According to REACH, log Kow tests are required for all substances produced with a tonnage above 1 Mg/year. If log Kow ≤ 3, then in accordance with Annex IX to REACH, no bioaccumulation studies are needed because the substance has a low potential for bioaccumulation. For the CLP classification, the limit value is log Kow ≥ 4, because above this value it is absolutely necessary to perform bioaccumulation tests. The n-octanol /water partition coefficient obtained in studies (2.1) means that Hydroxyester HE-1 has a low potential for bioaccumulation.

Table. 3. Results of physicochemical tests acc. to [ON8]

Type of test	Result	Unit
Melting point acc. to OECD guideline No. 102	no melting point in the temperature range from -60 °C do 20 °C	
Boiling point acc. to OECD guideline No. 103	255	°C
Relative density acc. to OECD guideline No. 109, at a temperature of 20 °C	0.9477	-
Solubility in water acc. to OECD guideline No. 105, at a temperature of 20±0,5 °C	972.06 (pH = 8,43)	mg/l
Partition coefficient of n- octanol /water acc. to OECD guideline No. 117	2,1	-
Flash point acc. to Regulation WE 440/2008	128	°C
Auto-ignition temperature Regulation WE 440/2008	410 (pressure = 1000 hPa)	°C
Viscosity acc. to OECD guideline No. 114, at a temperature of 20 °C	18.6	mm^2/s

For the assumed production scale in the range of 100 to 1000 Mg/year, six toxicological and 8 ecotoxicological tests are required. The results of these tests are presented in Tables 4 and 5. Based on the analysis of test results and requirements specified in the Regulation of the Minister of Health (2012), I determined the impact of Hydroxyester HE-1 on the environment and human health. The results of the required ecotoxicological tests are described in publications ON1 and ON3. In the case of toxicological tests, the results of skin irritation or corrosion tests, eye irritation and acute toxicity when exposed through the alimentary tract have been described in publications ON1 and ON3. However, in the case of skin sensitization and gene mutation studies in in vitro and mammalian in vitro mammalian cells, the results of the research were presented in the project "Commercialization of isobutyl aldehyde trimer manufacturing technology as a substitute for aromatic derivatives for the production of modern solvents and surfactants" carried out in 2007-2010 at the Opole University of Technology (Annex 3, point II.J.1).

Table 4. The impact of Hydroxyester HE-1 on human health

Lp.	Toxicological properties	Results
1.	Acute skin irritation/ corrosion study on rabbits acc. to OECD guideline No. 404	During test, erythema, swelling and drying of the epidermis were observed in the examined rabbits on exposed skin [ON1, ON3].
2.	Acute eye irritation/ corrosion study on rabbits acc. to OECD guideline No. 405	After giving of the test material during the experiment, slight changes in the cornea, iris and conjunctiva of the examined rabbits were observed [ON1].
3.	Skin sensitization acc. to the OECD guideline No. 406	During the test there were no allergic skin reactions on animals.
4.	Acute oral toxicity study on rats acc. to OECD guideline No. 420	During the 14-day duration of the experiment, no toxicity was observed. While macroscopic examination, no pathological changes were observed on animals [ON1].
5.	Bacterial reverse mutation test acc. to OECD guideline No. 471	The Hydroxyester HE-1 does not result in a statistically significant increase in the number of revertants depending on the dose or a statistically significant repetitive positive response to any of the test points.
6.	Gene mutation assay in mammalian cells in vitro according to OECD guideline No. 476	The HE-1 hydroxyester does not induce gene mutations in mammalian cells.

Based on the analysis of toxicological results (table 4), I found that Hydroxyester HE-1 is safe for human health. Only in the case of irritating and corrosive effects on the skin, the test result was negative during the first three days of the test, however, after 7 days of the skin test, only minor changes were visible. This means that when using the Hydroxyester HE-1, special care should be taken, especially in the skin contact.

Table 5. The impact of Hydroxyester HE-1 on water and soil environment [ON1, ON3]

Lp.	Ecotoxicological properties	Results
1.	Growth inhibition test. Pseudokirchneriella subcapitata, acc. to OECD guideline No. 201	The average concentration causing 50% inhibition of biomass increment (EyC_{50} /72h) is 48.10 mg /l, and the average concentration causing 50% inhibition of the average specific growth rate of algae culture at nominal concentrations of the tested product (ErC_{50} /72h) is above 80 mg /l [ON1].
2.	Daphnia Magna acute immobilization test acc. to OECD guideline No. 202	The average concentration causing 50% immobility of the Daphnia population (EC_{50} /48h) is above 100 mg /l, EC_0 /48h is equal to or above 100 mg /l, EC_{100} /48h is above 100 mg /l [ON1].
3.	Acute toxicity for rainbow trout acc. to OECD guideline No. 203	After 96 h of exposure, the LC_{50} value is 41 mg /l, LC_0 = 32 mg /l and the LC_{100} value = 56 mg /l [ON1].
4.	Acute toxicity to earthworms acc. to OECD guideline No. 207	The highest concentration used in the experiment, which causes no mortality of earthworms (LC_0) after 7 days of experiment, is 560 mg /kg, while after 14 days it is 320 mg /kg of dry matter of artificial medium. The lowest concentration causing 100% mortality (LC_{100}) after 7 and 14 days of experiment is 1000 mg/kg of artificial medium [ON1].
5.	Activated sludge respiration inhibition test acc. to OECD guideline No. 209	The Hydroxyester HE-1 concentration causing 50% inhibition of activated sludge breathing rate (EC_{50}) was 608.45 mg /dm^3 [ON1].
6.	Soil microorganisms: nitrogen transformation test acc. to OECD guideline No. 216	Based on the obtained results, it was found that: - EC_{50} - the concentration of the tested material in the soil causing 50% inhibition of nitrogen transformation to nitrates after 28 days is 444.2 mg /kg of soil, - EC_{25} - the concentration of the tested material in the soil causing 25% inhibition of nitrogen transformation to nitrates after 28 days is 278.7 mg /kg of soil, - EC_{10} - the concentration of the tested material in the soil causing 10% inhibition of nitrogen transformation to nitrates after 28 days is 182.8 mg / kg of soil [ON1, ON3].
7.	Soil microorganisms: carbon transformation test acc. to OECD guideline No. 217	Based on the obtained results, it was found that: - EC_{50} - the concentration of the tested material in the soil causing 50% inhibition of carbon to carbon dioxide transformation after 28 days is greater than 1000 mg /kg of soil,

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		- EC_{25} - the concentration of the tested material in the soil causing 25% inhibition of carbon to carbon dioxide transformation after 28 days is greater than 1000 mg /kg of soil, - EC_{10} - the concentration of the tested material in the soil causing 10% inhibition of carbon to carbon dioxide transformation after 28 days is greater than 1000 mg /kg of soil [ON1].
8.	Ready biodegradability, closed bottle test acc. to OECD guideline No. 301	After 28 days of experiment, the biodegradation value of the tested material was 61.9%. Since the biodegradation of the Hydroxyester HE-1 after 28 days was above 60%, it was found that the tested product is biodegradable [ON1].

According to the Regulation of the Minister of Health (2012), a chemical substance is safe for the aquatic and soil environment when the concentration is above 100 mg /dm^3. Presented results indicate that the Hydroxyester HE-1 is a safe product for the water and soil environment. Only in the case of rainbow trout and the growth of algae biomass, Hydroxyester HE-1 may be toxic, but only at higher concentrations.

Iron-based combustion modifier for liquid fuels

Physicochemical properties play a key role in assessing the behavior of chemical substances in the environment, and were therefore necessary to determine the risk of an iron additive to assess the impact.

Eight physicochemical properties of the modifier were made, which was resulted from the adopted production volume (Table 6). The tests were carried out in accordance with the OECD guidelines and European Community regulations.

Table 6. Results of physicochemical tests [ON6]

Type of test	Result	Unit
Physical state at 20 °C and pressure of 101.3 kPa	liquid	-
Boiling point	277 (±22)	°C
Relative density	0.9071 (±0,001)	g/cm^3
Solubility in water at a temperature of 20°C ± 0.5	Baze oil: 132.3 Iron salts: 47.6	mg/dm^3
Partition coefficient of n- octanol / water	no marking	
Flash point	94 (±2)	°C
Auto-ignition temperature	250 (±6) p=990.5 hPa	°C
Kinematic viscosity at a temperaturę of 20° C	11.89	mm^2/s

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Based on the obtained test results, it was found that the boiling point of the iron-based combustion modifier for liquid fuels is over 270 ° C. Ignition and auto-ignition temperatures are 94 and 250 ° C, respectively.

For the iron-based combustion modifier for liquid fuels, 8 toxicological (Table 7) and 10 ecotoxicological tests were performed (Table 8), which in the same way as in the case of Hydroxyester HE-1 were selected on the basis of the planned production volume and guidelines of the REACH regulation. The obtained results were compared with the requirements of the Regulation of the Minister of Health (2012), and on this basis it was possible to determine the impact of the iron-based combustion modifier for liquid fuels on the environment and human health. I presented the results of the tests in Tables 7 and 8.

Table 7. Toxicological test results for iron-based modifier

Lp.	Toxicological properties	Results
1.	Acute dermal toxicity study on rats acc. to OECD guideline No. 402	The median lethal dose of skin (LD_{50}) for the test material is greater than 2000 mg /kg m.c.
2.	Acute skin irritation/ corrosion study on rabbits acc. to OECD guideline No. 404	The mean value of the point score of erythema forming after 24, 48 and 72 hours (for three rabbits) was 2.66, while in the case of edema the mean value was 1.23 [ON10].
3.	Acute eye irritation/ corrosion study on rabbits acc. to OECD guideline No. 405	After giving the iron modifier, no changes were observed in the cornea and iris of the eye, only changes in the conjunctiva of the eye were observed, which were only transient in nature. The average after 24, 48 and 72 hours was for the conjunctiva (for three rats), in the case of erythema 0.9, and for edema 0,2 [ON4].
4.	Skin sensitization acc. to the OECD guideline No. 406	After giving the iron modifier to the skin of the exposed animals, no allergic changes were observed [ON4].
5.	Acute oral toxicity study on rats acc. to OECD guideline No. 420	After giving a single dose of the test material in the volume of 2000 mg / kg m.c. to the five animals in the initial and actual experiment, animals showed no signs of toxicity. All animals survived the experiment period [ON10].
6.	In vitro skin corrosion: transcutaneous electrical resistance test acc. to OECD guideline No. 430	The iron modifier can be classified as corrosive / severely irritating material. The average OES values for the tested material were above 5 kΩ, and no pathological changes were found on the skin discs.
7.	Isolated chicken eye test method for identifying ocular corrosives and severe irritants acc. To OCED guideline No. 438	The average degree of fluorescein retention for the eyes exposed to the test material was 2.0 (III Class ICE). However, the average degree of corneal opacity for eyes exposed to the tested material was 2.0 (III Class ICE). In turn, no corneal edema (ICE Class I) was found for eyeballs exposed to the test material. According to the Joint

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		Classification of Irritant Action of ICE in vitro, it can be stated that the examined material has not shown any damaging effects on the eye [ON10].
8.	Bacterial reverse mutation test acc. to OECD guideline No. 471	The iron-based modifier has no mutagenic effect on the used bacterial strains.

Despite the same planned tonnage of production as in the case of the Hydroxyester HE-1, for the iron-based combustion modifier for liquid fuels, it was decided to perform two more toxicological and ecotoxicological tests. In the case of toxicological tests, an acute skin toxicity test was carried out according to the OECD guideline No. 402 and an in vitro skin corrosion test according to the OECD guideline No. 430. This is related to the fact that iron in large quantities may negatively affect human health, as described in the ON10 publication. In the case of ecotoxicological studies, an additional study was carried out on the emergence and growth of terrestrial plants, according to the OECD guideline No. 208 and Daphnia magna reproduction test (OECD guideline No. 211). As this was shown in publication ON9, iron in large quantities negatively influences on the aquatic and on the soil environment.

Most of the results of required toxicological tests are described in publications ON4 and ON10. In the case of acute skin toxicity tests, in vitro skin corrosion effects and in vitro bacterial gene mutation tests, the results of the research have been presented in the project entitled: "Research on the energy-ecological efficiency system for burning solid and liquid fuels" carried out in 2012-2014 at West Technology & Trading Polska SA and Opole University of Technology (Annex 3, point II.J.3).

Analysis of the obtained results of toxicological tests under the requirements of the Regulation of the Minister of Health (2012) indicates that the iron-based combustion modifier for liquid fuels is safe for human health. Only in the case of irritating and corrosive effects on the skin, the result of the test does not meet the guidelines of the Regulation. This means that when using the iron-based combustion modifier for liquid fuels, special care should be taken, especially in the skin contact.

The results of ecotoxicological studies have been described in the works ON4, ON5, ON6 and ON9. In the case of acute toxicity for earthworms, the results of the research were presented in the project as above (Annex 3, point II.J.3).

Table 8. Ecotoxicological test results for iron-based modifier

Lp.	Ecotoxicological properties	Results
1.	Growth inhibition test. Pseudokirchneriella subcapitata, acc. to OECD guideline No. 201	The average concentration causing 50% inhibition of algae growth in EyC_{50}/72 h was 26.59 mg/dm^3. The value of the lowest concentration of the tested material causing the LOEC/72 h biomass inhibition effect is 10.0 mg/dm^3, while the highest concentration of the test material not causing the NOEC effect/72 h was 3.2 mg/dm^3 [ON9].

2.	Daphnia Magna acute immobilization test acc. to OECD guideline No. 202	The average concentration causing the immobility of the daphnia, that is, the inability to swim in 50% of individuals after 48 hours of exposure is 0.84 mg/l [ON4].
3.	Acute toxicity for rainbow trout acc. to OECD guideline No. 203	The LC_{50} value after 96 h of exposure was 166.94 mg /dm^3, which according to the Regulation of the Minister of Health (2012) means that the iron modifier does not adversely affect rainbow trout [ON9].
4.	Acute toxicity to earthworms acc. to OECD guideline No. 207	After using iron modifier, in concentrations from 100 to 1000 mg/kg dry weight of the artificial substrate, the weight loss of earthworms was found in relation to the initial mass in the range from 12.7 to 18.4%. On the other hand, in control earthworms, a body mass loss of 14.8% was also observed.
5.	Terrestrial plant test: seedling emergence and seedling growth test acc. to OECD guideline No. 208	There was no delay in plant emergence compared to the control group. However, based on the measurement of the length and dry matter of the shoots, it was found that the test material causes the inhibition of growth of all tested plant species. Among the symptoms of phytotoxic activity, inhibited growth and deformation of plants were observed. These symptoms were most pronounced after using iron modifier in concentrations of 500 and 1000 mg/kg of dry soil [ON5].
6.	Activated sludge respiration inhibition test acc. to OECD guideline No. 209	In the experimental conditions and in the applied concentration range from 100 to 1000 mg/l, the tested material does not inhibit the respiration of activated sludge microorganisms. In turn, the concentration of the test material at which 50% breathing inhibition of activated sludge microorganisms (EC_{50}) occurs is higher than 1000 mg/l [ON4].
7.	Daphnia magna reproduction test acc. to OECD guideline No. 211	There was no negative effect of the test material on reproduction, immobility, body length and age of reproduction. As a result of the study of the effect of iron modifier concentration on daphnia proliferation, a reduction in their reproduction was observed from 0.6% to 16.7%, depending on the nominal concentration [ON9].
8.	Soil microorganisms: nitrogen transformation test acc. to OECD guideline No. 216	Iron modifier in concentrations from 125 to 2000 mg/kg of soil does not inhibit the transformation of nitrogen to nitrates, and carbon to carbon dioxide [ON5].
9.	Soil microorganisms: carbon transformation test acc. to OECD guideline No. 217	Iron modifier in concentrations from 125 to 2000 mg/kg of soil does not inhibit the transformation of nitrogen to nitrates, and carbon to carbon dioxide [ON5].

10.	Ready biodegradability, closed bottle test acc. to OECD guideline No. 301	Biodegradation on 7th day was 30.65%, 44.66% on 14th day, 57.80% on the 21th day and 62.18% on the last day of the experiment. On the basis of the Regulation of the Minister of Health (2012), it can be concluded that the iron modifier readily breaks down in the water environment [ON6].

Because according to the Regulation of the Minister of Health (2012), a chemical substance is safe for the aquatic and soil environment when the concentration is above 100 mg /dm^3, most of the research results indicate that the iron-based combustion modifier for liquid fuels is safe for the water and soil environment. However, at higher concentrations, the iron-based combustion modifier for liquid fuels may negatively affect the growth of algae biomass, as well as may immobilize daphnia.

4.4.3. Assessment of the applicability of QSAR methods to determine the impact of Hydroxyester HE-1 and iron-based combustion modifier for liquid fuels on the environment and human health

In order to assess the applicability of the quantitative relationship between chemical structure and biological activity to determine the impact of chemical substances on the environment and human health, I compared the selected results of experimental studies presented in section 4.4.2. with results obtained from the use of various QSAR tools. For Hydroxyester HE-1, I identified physicochemical properties such as melting point, boiling point, flash point, viscosity, solubility in water and density. To determine these properties, I used the Toxicity Estimation Software Tool (T.E.T.) [ON8]. The n-octanol/water partition coefficient which is necessary to determine the biological activity of the compound was determined using the Vega in silico platform [ON7]. In contrast, for the iron-based combustion modifier for liquid fuels I determined the selected ecotoxicological properties using the T.E.S.T. [ON11]. All QSAR tools are based on databases on chemical compounds. Therefore, the chemical compound we want to find is not always present in this database and not all information about the impact of this compound on the environment and human health are included there. The largest number of physicochemical information of the Hydroxyester HE-1 I found in the software T.E.S.T. However, in the case of the n-octanol/water partition coefficient, much information (up to three models) was found in the Vega in silico platform. It was much more difficult to select the QSAR tools for a multicomponent substance - an iron-based combustion modifier for liquid fuels. Because this substance is the reaction mass of 4 components, only for the software T.E.S.T. it was possible to evaluate all four components.

Hydroxyester HE-1

To assess the physicochemical properties of the Hydroxyester HE-1, I used the T.E.S.T tool, because from the analysis of the obtained results for all commonly available software, which I presented in Table 1, the most information concerns physicochemical properties. The T.E.S.T tool allows to estimate toxicological and ecotoxicological properties using several different advanced QSAR methodologies also (Martin et al., 2008). The following methods have been used to determine the physicochemical properties and toxicity of the Hydroxyester HE-1:

• Hierarchical method: Toxicity for a test compound is estimated using the weighted average prediction from several different models. The genetic algorithm technique is used to generate models for each group of compounds.

• FDA method: The prediction of each result is made using a new model that matches the substances most closely related to the test compound.

• Single model method: Predictions are made using the MLR model and molecular descriptors, as independent variables, using the genetic algorithm.

• Group contribution method: predictions are made using a multilinear regression model by the number of molecules as independent variables.

• Nearest neighbor method: Predicted toxicity is estimated based on the average of results obtained for three chemical substances most closely related to the test substance.

A very important element in assessing the effectiveness of each QSAR tool is determining the reliability of the obtained result based on the similarity of the compounds. T.E.S.T. tool calculates a similarity coefficient from 0 (in the case of 0% compliance) to 1 (100% compliance). Typically, values lower than 0.75 indicate that a similar compound shows significant differences compared to the test compound (Floris et al., 2014). In this case, it should be consider whether the chosen tool is appropriate and possibly look for another one.

To assess the compatibility of the models, I used the root-mean square error (RMSE) and mean absolute error (MAE) which were calculated according to equations (1) and (2):

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n}} \quad (1)$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \quad (2)$$

where:

y_i – the value obtained during experimental research,

$\hat{y}_i$ – value obtained using the QSAR methods,

n – number of tested substances [ON8].

The applied QSAR model is considered as satisfactory when the root-mean square error is as close to zero as possible.

In table 9, I presented the results of the physicochemical properties calculated for Hydroxyester HE-1 using the T.E.S.T. tool. I combined the results of melting point, boiling point, density, water solubility, ignition temperature and viscosity depending on the used QSAR method. The analysis of the test results shows that depending on the applied QSAR method, the determined values of physicochemical properties differ significantly, therefore for the further analysis of the test results I used the mean values taking into account the results determined by different QSAR methods. The solubility in water and viscosity are given in logarithmic values. After conversion to the commonly used quantities, these values were respectively 1524,91 mg/L and 8,68 cP.

Table 9. Results of physicochemical properties for Hydroxyester HE-1, determined using the T.E.S.T tool [ON8]

Method	Melting point, °C	Boiling point, °C	Density, g/cm³	Solubility in water - log_{10}(mol/L)	Ignition temperature, °C	Viscosity, Log_{10}(cP)
Hierarchical	20,13	247,50	0,94	2,53	95,39	0,96
FDA	43,91	223,35	0,99	2,08	115,01	1,07
Single model	-	-	-	-	-	0,51
Group contribution	-30,44	261,42	0,84	2,54	92,76	1,18
Nearest neighbor	27,03	266,30	0,92	1,47	115,01	0,97
Average value	15,16	249,64	0,92	2,15	104,83	0,94

On Figure 2, I compared the results of experimental studies (derived from various databases) with the results obtained using the T.E.S.T. tool, for substances with a similar structure to the Hydroxyester HE-1. The coefficient of structural similarity for these substances ranged from 0.51 to 0.79. This means that some compounds have significant differences compared to the Hydroxyester HE-1 and these results may not be completely reliable.

On the graphs (Fig. 2), I placed the average absolute error (MAE), depending on the tested property. I observed that the best compatibility was obtained for boiling point and density. However, the biggest differences in results were noted for solubility in water and viscosity.

I drew very similar conclusions by comparing the results of my own research for the Hydroxyester HE-1 (Table 3) with the results from the T.E.S.T. tool (Table 10). To assess the conformity between the results of my own tests and the results from the T.E.S.T tool, I used a relative error calculated according to the formula (3):

$$\delta_y = \frac{|y_i - \hat{y}_i|}{y_i} \cdot 100\% \quad (3)$$

where:

y_i - the value obtained during experimental research,

$\hat{y}_i$ - value obtained using the QSAR methods.

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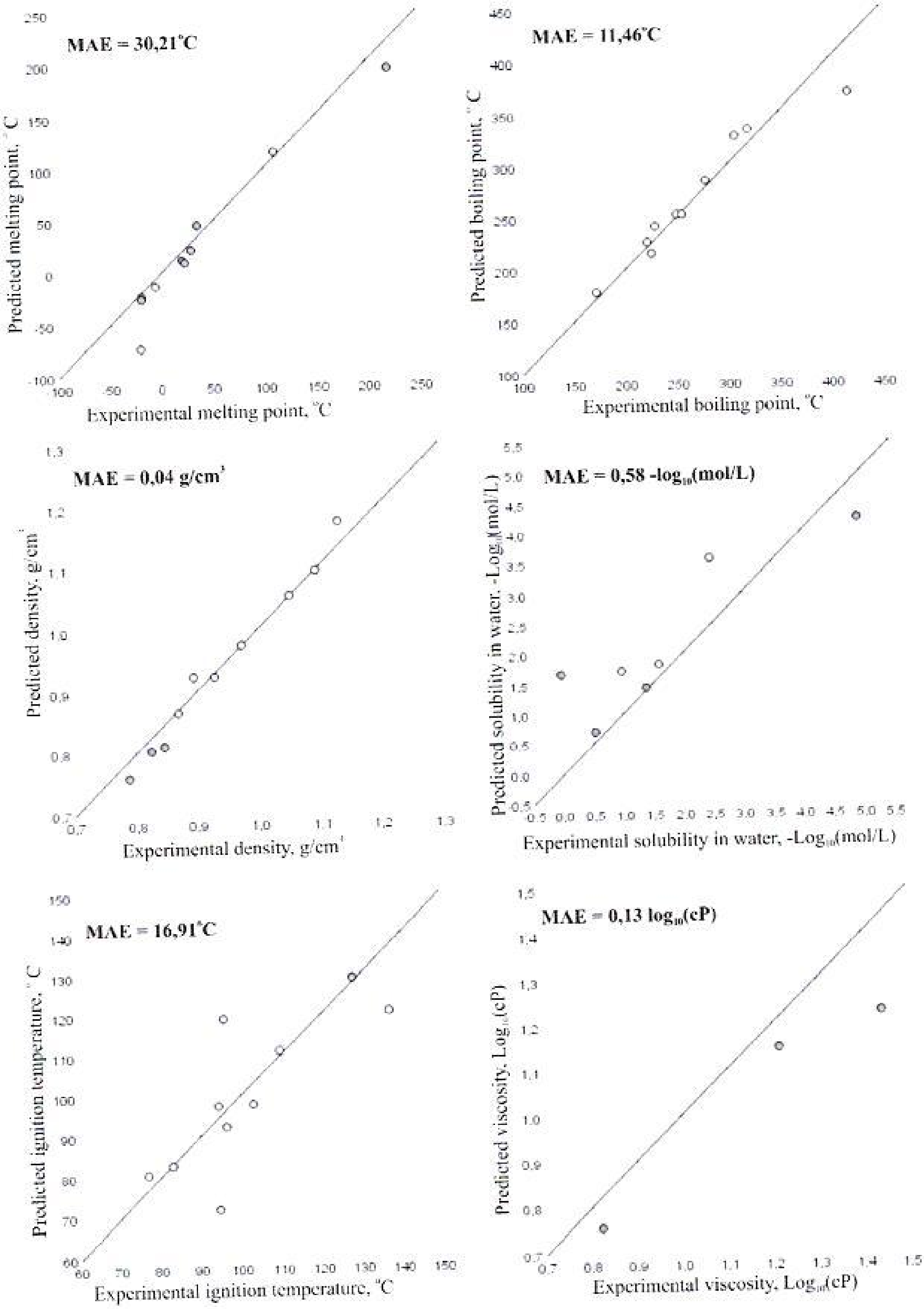

Figure 2. Comparison of experimental results with results from the T.E.S.T. tool, for substances of similar structure to Hydroxyester HE-1 [ON8]

I have observed that the smallest relative error (2.1%) was noted for the boiling point. The obtained result (249.64 °C) indicates that Hydroxyester HE-1 is a volatile organic compound (VOC). However, based on the own performed tests, the boiling point was 255 °C, which indicates that Hydroxyester HE-1 is not VOC.

Good compatibility was also obtained for density, the error in this case was only 2.9%. In the case of solubility in water and viscosity tests, the T.E.S.T. tool did not work, because the relative error is high and in both cases it was over 50%.

Table 10. Comparison of experimental results and from the T.E.S.T. for Hydroxyester HE-1 [ON8]

Properties	**Experimental results**	**T.E.S.T. tool**	**Relative error, %**
Melting point	no melting point in the temperature range from -60 °C do 20 °C	15,16 °C	undefined
Boiling point	255 °C	249,64 °C	2,1
Density	0,9477 g/cm³	0,92 g/cm³	2,9
Solubility in water	972,06 mg/L	1524,91 mg/L	56,9
Ignition temperature	128 °C	104,83 °C	18,1
Viscosity	17,627 cP	8,68 cP	50,76

The biggest differences between the results of own research and the results from the T.E.S.T. tool occur in the case of determining the melting point. In this case, the average melting temperature determined with T.E.S.T. differs significantly from the result of experimental research. These tools are therefore not suitable for such a test, which is also confirmed by the comparison of experimental results with results from the T.E.S.T. tool for substances with a similar structural structure to Hydroxyester HE-1, shown in Fig. 2. In this case the MAE value was 30.21 °C.

In order to determine the value of the partition coefficient n-octanol/water (log P), the Vega in silico platform was used because it contains the largest number of models used to determine this coefficient [ON9].

In publication [ON7] I compared the results of own research determining the n-octanol /water partition coefficient for the Hydroxyester HE1 (Table 3) with the results obtained using different QSAR methods. To determine the value of log Kow, I used three available models from the VEGA in silico tool: Kowwin, MlogP and AlogP. To assess the results obtained by these models, I used the root-mean square error (RMSE) - formula (1), and the determination coefficient (R^2), calculated according to the formula (4):

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i-\hat{y}_i)^2}{\sum_{i=1}^{n}(y_i-y_{avg})^2} \quad (4)$$

where:

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y_{avg} – average of all values using QSAR methods.

The applied QSAR model is considered as satisfactory when the determination coefficient is equal or as close as possible to unity.

On Figure 3, I compared the results of experimental studies (coming from different bases) with the results obtained using the VEGA platform for substances of similar structure to Hydroxyester HE-1. The obtained results can be considered reliable because the similarity coefficient ranged from 0.805 to 0.878. For each of the three used models, the determination coefficient (R^2) and the root-mean square error (RMSE) were calculated. The determination coefficient for all three used models was satisfactory and was successively: MlogP - 0.9878, AlogP - 0.9596 and for Kowwin - 0.9718. In turn, the average square error for the MlogP model was the highest and amounted to 1.03, for the AlogP model it was 0.72, and for Kowwin = 0.39. Based on the analysis of the obtained results, I found that, taking into account the molecular similarity, the best models for determining the division coefficient n-octanol/water are in the order: Kowwin, AlogP, MlogP.

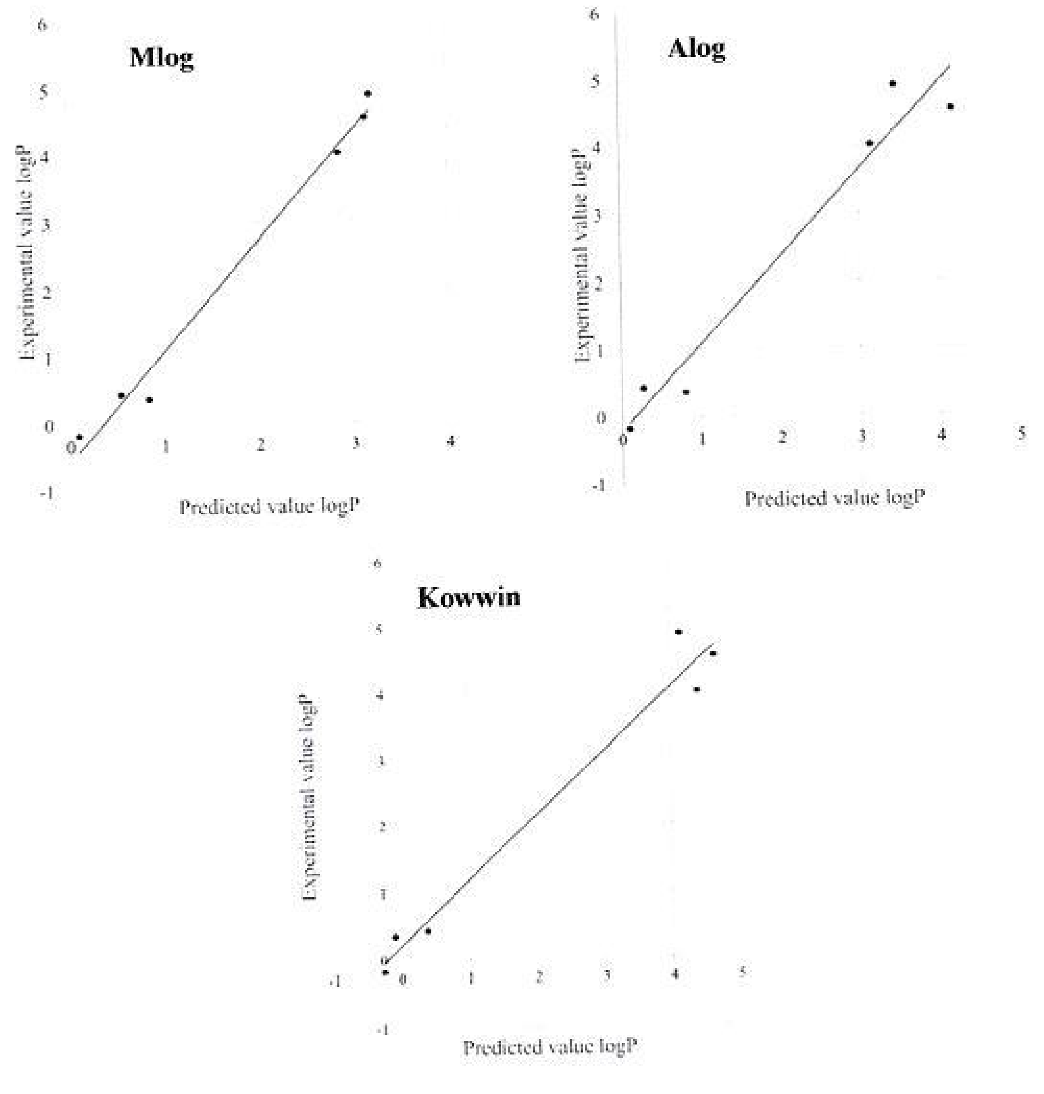

Figure 3. Comparison of experimental results with results using models: MlogP, AlogP and Kowwin for substances with similar structure to Hydroxyester HE-1 [ON7]

Then for each of the three models I calculated the average value of logP (mean of 6 values obtained for compounds with molecular similarity) and compared with the value obtained during own research (logP = 2.1), as well as calculated the relative error (Table 11). The best compatibility between the results of own research and those from the QSAR models were obtained consecutively for the models: AlogP, MlogP, Kowwin.

Table 11. Comparison of logP average values from various QSAR models with the value derived from own research for Hydroxyester HE-1 [ON7]

Method	logP	Relative error, %
Own research	2,1	-
MlogP	2,75	30,9
AlogP	2,42	15,2
Kowwin	3	42,8

Comparing the results of the tests presented in Figure 3 and Table 11, it can be concluded that in the case of the n-octanol/water partition coefficient the best compatibility between the results of own tests and those derived from QSAR tools was obtained for the AlogP model.

Iron-based combustion modifier for liquid fuels

An example of the evaluation of the possibility of using QSAR methods to analyze the impact of chemical substances on the environment and human health is the use of the T.E.S.T. tool to determine the effect of an iron-based combustion modifier for liquid fuels on the environment [ON11]. Compared to the Hydroxyester HE-1, iron modifier is a much more difficult compound to evaluate in QSAR tools. This is due to the fact that it is a reaction mass consisting of: iron soap in the form of iron (III) palmitate and iron (III) stearate, iron (III) hydroxide and heating oil. Therefore, it was very difficult to select the right tool and properties to get data for all four components of the reaction mass. Thus, for the iron modifier I selected three ecotoxicological properties evaluated using the T.E.S.T. tool.

In the work [ON11], to assess the ecotoxicological properties of the modifier, I used the latest VEGA in silico platform version 1.1.4, available at www.vega-qsar.eu. The input signal was an unambiguous record of the structure of molecules of chemical compounds using the string of characters - smiles.

In Table 12 I have compiled the smiles for all four components of the iron modifier reaction mass.

In the cited work [ON11], I analyzed the following properties using available QSAR models: rainbow trout toxicity study (LC_{50}/96h) using the EPA v.1.0.7 model, Daphnia immobilization (EC_{50}/48h) used models: EPA v.1.0. 7 and DEMETRA v.1.0.4, ready biodegradation using the IRFMN v.1.0.9 model.

The results of laboratory tests for the iron modifier and the results from the VEGA in silico platform for the four main components of reaction mass are presented in Table 13. In addition, in the table the values of concentrations which are safe for the environment in accordance with the Regulation of the Minister of Health were included (2012).

Table 12. Names, CAS numbers, formulas and the smiles of iron modifier

Name of compound	CAS number	Formula	Smiles
Iron (III) palmitate	20259-32-9	$C_{48}H_{93}FeO_6$	CCCCCCCCCCCCCCCC(=O)OCCCC CCCCCCCCCCCC(=O)OCCCCCCCC CCCCCCCC(=O)O[Fe]
Iron (III) stearate	555-36-2	$C_{54}H_{105}FeO_6$	CCCCCCCCCCCCCCCCCC(=O)OCC CCCCCCCCCCCCCCCC(=O)OCCCC CCCCCCCCCCCCCC(=O)O[Fe+3]
Iron (III) hydroxide	1309-33-7	FeH_3O_3	O[Fe](O)O
Heating oil	68334-30-5	$C_{92}H_{182}$	CCC(C)C(CCC(C)C(C)C)C(C)CCCCC CCC(CC)C1=CC(CCC)=CC=C1CCCC CCCCCCC1CC(CCC(C)CCC)C(C1)C (C)CCCCCCCCCCCCCCCCCCCCC CCCCCCCCCCCCC

The results of laboratory tests indicate that the iron modifier defined as a reaction mixture consisting four substances has a negative effect on daphnia, does not toxically affect rainbow trout and is biodegradable.

The VEGA tools were tested separately for each substance included in the iron modifier, because there is no equivalent for such a mixture in the database.

In the daphnia immobilization test, using VEGA in silico tool, I observed that for the iron (III) palmitate, iron (III) stearate and fuel oil EC_{50} values close to zero were obtained (Table 13). In the case of iron (III) hydroxide, the results obtained for two models are 2.97 mg/dm^3 and 7.38 mg/dm^3, respectively. According to the Regulation of the Minister of Health (2012), if the EC_{50} value after 48h of exposure is less than or equal to 10 mg/dm^3, the substance may cause long-term adverse changes in the aquatic environment and be toxic to aquatic organisms. On the other hand, in the laboratory tests for iron-based modifier, the EC_{50} value = 0.84 mg/dm^3 was obtained in the test of acute immobility of daphnia. The results of laboratory tests and using the Vega platform indicate that both the mixture and the iron modifier components affect on daphnia. Comparing the above results, I found compatibility between laboratory methods and QSAR methods.

In an acute toxicity test for rainbow trout using the VEGA in silico tool, I observed that for iron (III) palmitate, iron (III) stearate and fuel oil, LC_{50} values close to zero were obtained, which means that these compounds negatively affect the fish. However, in the case of iron (III) hydroxide, the determined LC_{50} value many times exceeds the limit value and amounts to

9618,27 mg/dm^3, which according to the Regulation of the Minister of Health means that the tested compound does not adversely affect the rainbow trout and is safe for the aquatic environment.

Table 13. Results of laboratory tests and from VEGA in silico platform for the evaluation of the ecotoxicological properties of the iron modifier

	***Daphnia magna* immobilization test**	**Acute toxicity study for rainbow trout**	**Ready biodegradability**
Concentration safe for an environment	> 100 mg/dm^3	> 100 mg/dm^3	BOD > 60%
Iron-based modifier*	EC_{50} = 0,84 mg/dm^3	LC_{50} = 166,96 mg/dm^3	BOD = 62,18%
Results from the VEGA in silico platform for the four main components of the reaction mass			
Iron (III) palmitate	EC_{50} = 10,13 – log(mol/dm^3) – about 0 mg/dm^3 (DEMETRA v.1.0.4) EC_{50} = 11,1 – log(mol/dm^3) – about 0 mg/dm^3 (EPA v.1.0.7)	LC_{50} = 13,53 – log(mol/dm^3) – about 0 mg/dm^3	biodegradable
Iron (III) stearate	EC_{50} = 9,79 – log(mol/dm^3) – about 0 mg/dm^3 (DEMETRA v.1.0.4) EC_{50} = 11,78 – aboutlog(mol/dm^3) – about 0 mg/dm^3 (EPA v.1.0.7)	LC_{50} = 15,13 – log(mol/dm^3) – about 0 mg/dm^3	biodegradable
Iron (III) hydroxide	EC_{50} = 2,97 mg/dm^3 (DEMETRA v.1.0.4) EC_{50} = 7,38 mg/dm^3 (EPA v.1.0.7)	LC_{50} = 9618,27 mg/dm^3	no data
Heating oil	EC_{50} = 9,84 – log(mol/dm^3) – about 0 mg/dm^3 (DEMETRA v.1.0.4) EC_{50} = 13,92 – log(mol/dm^3) – about 0 mg/dm^3 (EPA v.1.0.7)	LC_{50} = 25,51 – log(mol/dm^3) – about 0 mg/dm^3	not biodegradable

* - laboratory tests

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In the case of laboratory tests for the iron-based modifier being the mixture, the LC_{50} value was obtained = 166.96 / dm^3, which also indicates that the tested iron-based modifier does not adversely affect rainbow trout. Comparing the results of laboratory tests with the results from the VEGA in silico tool, I observed that in the case of the QSAR tool, the most important impact on acute toxicity for rainbow trout had iron (III) hydroxide. Only in this one case the obtained result confirmed laboratory tests for the iron modifier. On the other hand, the average result for the four components of the mixture determined according to the VEGA tools is higher than the safe concentration, which to some extent is consistent with the results of laboratory tests for the mixture of ingredients.

In the case of ready biodegradability tests, the results obtained with the VEGA tools for iron (III) palmitate and iron (III) stearate indicate that they are biodegradable. In turn, heating oil is not biodegradable, and for iron (III) hydroxide in available bases I have not found obtained data. Because, according to the results of laboratory tests, the iron-based modifier is biodegradable (BOD = 62.18%), I found that from four components of the reaction mass the most important for biodegradability are iron (III) palmitate and iron (III) stearate. In these two cases, the obtained results confirmed the laboratory test results for the iron modifier.

In addition, based on the final reports generated by the VEGA in silico tool for the four components of reaction mass, I determined the reliability of the obtained results. For the four tested components, the similarity factor in the ready biodegradability test ranged from 0.5 to 0.74. The lowest structural similarity coefficient was obtained for compounds with a similar structure to heating oil, and was in the range of 0.5 - 0.52. However, the highest structural similarity coefficient (0.74) was obtained for iron (III) palmitate and iron (III) stearate. To consider the result as satisfactory, the similarity coefficient should be in the range from 0.75 to 1. The determined reliability of the result was not the best and further works are necessary to improve the tool or find a better one.

4.4. The importance and possible uses of results

Research on the assessment of the applicability of the quantitative relationship between the chemical structure and biological activity of two environmentally friendly products, the results of which have been published in the publication cycle discussed above, are of great scientific and practical importance in two aspects. First of all, in terms of innovative products that are safe for the environment, and secondly, limitations of animal tests. From a scientific point of view, the obtained results are an extension of our knowledge about non-invasive methods of assessing the impact of chemical compounds on the environment and human health. From a utilitarian point of view, they help reduce costly animal testing and help to expand the range of technical solutions that are useful in solving environmental engineering problems. This pragmatic aspect is of particular importance when using QSAR methods in research aimed at registering safe products on the European Union market under the REACH Regulation. These studies both in Poland and in the world are still a big challenge and require looking for sustainable solutions.

The most important result of the described research is the possibility to apply methods of quantitative relationship between chemical structure and biological activity, to assess the impact of chemical compounds on the environment and human health. Although as described in section 4.4.3, the compatibility between the experimental results (point 4.4.2) and the QSAR tools is not always satisfactory, I think that these methods are forward-looking. The research results and their analysis indicate that currently QSAR methods can be used primarily to determine boiling point, relative density and n-octanol/water partition coefficient. Although they are physicochemical properties of the substance, they provide much needed information about the behavior of substances in the environment. On the other hand, the analysis of results indicates that in the case of determination of toxicological and ecotoxicological properties for compounds with a complex structure, the compatibility between experimental studies and the results of QSAR methods is not the best. An example of a such substance is the iron-based combustion modifier for liquid fuels, which is the reaction mass of four components being organic and inorganic compounds. However, these methods are developing rapidly and for sure in the near future, this compatibility will be sufficient and it will be possible to replace animal testing with research using QSAR models.

Another important result of the described research is my participation in the development of two technologies of environmentally friendly products, i.e. Hydroxyester HE-1 and iron-based combustion modifier for liquid fuels, for which production is planned in the amount of 100 to 1000 Mg/year (section 4.4.1). The advantages of these products are innovation and reduction of emissions of harmful substances into the atmosphere. Hydroxyester HE-1, due to the fact that it is not classified as a volatile organic compound, can replace toxic coalescents of paints and varnishes. In turn, the iron-based combustion modifier for liquid fuels, as presented in section 4.4.1, reduces the emission of harmful products of liquid fuels combustion into the atmosphere, as well as increases the efficiency of the boiler and reduces the amount of deposits on the grate and in the combustion chamber.

Generally, the scientific goal defined in Chapter 4.3.2 has been achieved, because as a result of the performed research, the usefulness of quantitative relationship between chemical structure and biological activity to assess the impact of chemical substances on the environment and human health has been demonstrated. The research also showed the imperfection of QSAR methods for assessing the impact of multicomponent compounds on the environment, which encourages further research and analysis in the future.

In addition to the implementation of the set scientific goals, it is worth emphasizing the scientific and practical significance of the discussed achievement. The performed research has a unique character on a global scale, contributing to the extension of our knowledge on this current topic. It is particularly valuable to analyze the use of QSAR methods to assess the impact of chemical compounds on the environment and human health under the REACH Regulation. In addition, it is also worth to notice that in the case of two described environmentally friendly products, their production is planned.

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5. Discussion of other scientific and research achievements

5.1. Before obtaining a doctoral degree

After graduating in 2004 a Master's degree in Environmental Engineering, I started a four-year PhD Studies at the Faculty of Mechanical Engineering at the Opole University of Technology. The subject of my PhD thesis concerned the influence of geometrical parameters on two-phase gas-liquid flow in the exchanger with baffles. As part of the work, I built a test stand where I analyzed the influence of many parameters, such as distance between baffles, relative scale, size of the cut-out, on the flow of a two-phase mixture in the tube bundle space of heat exchanger using image anemometry. The test results conducted in this time were presented at 10 conferences (Annex 3, point III.B.1-14) and published in 3 articles:

- **Guziałowska J.,** Ulbrich R., 2006, Badania hydrodynamiki przepływu mieszaniny gaz - ciecz w przestrzeni międzyrurowej z przegrodami poprzecznymi. W: Wykorzystanie metod analizy obrazu do oceny nierównomierności przepływu w elementach płaszczowo - rurowego wymiennika ciepła. Opole: Ofic. Wydaw. PO 2006, 123-139.

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- Ulbrich R., Siejka K., **Guziałowska J.,** Zając D., Karaś M., 2008, Wybrane problemy przepływu mieszaniny dwufazowej wokół pęku rur, W: Wybrane zagadnienia przepływu płynów i wymiany ciepła. Warszawa, 177-200.

After obtaining a doctoral degree I published two more publications in this subject:

- **Guziałowska J.**, Skoczylas D., Ulbrich R., 2009, Zastosowanie metod korelacyjnych w badaniach przepływu dwufazowego gaz-ciecz w przestrzeni międzyrurowej wymiennika ciepła, Inżynieria i Aparatura Chemiczna, 6, 78-80.
- Skoczylas D., **Guziałowska J.**, 2009,Parametry geometryczne a rozpływ płynu w pęku rur, Inżynieria i Aparatura Chemiczna, 6, 172-173.

In 2005, as part of the Socrates-Erasmus program, I took part in a three-month practice at the Institute of Process Engineering at the University of Hannover, where I deepened my knowledge of multi-phase flow.

During my doctoral studies I received a doctoral scholarship from the Marshal of the Opolskie Voivodeship for my progress in research.

5.2. After obtaining the doctoral degree

After obtaining the doctoral title, I was employed as an assistant at the Department of Environmental Engineering at the Faculty of Mechanical Engineering at the Opole University of Technology. Because I was employed in the team: "Waste management and chemical technology", my scientific and publication activity focused on three main research areas:

- the impact of chemical substances on the environment and human health as part of REACH registration,
- the use of oleochemical raw materials for the production of environmentally friendly products,
- waste management and sewage sludge.

The impact of chemical substances on the environment and human health as part of REACH registration

The most important area of my scientific activity was the assessment of the impact of new proecological solutions on the environment and human health. In particular, I worked on the use of experimental methods and QSAR tools to assess the safety of new chemical substances.

Even during the doctoral studies I worked on the chemical safety assessment of the substance, on the example of the Hydroxyester HE-1, as a part of the project implemented at the Opole University of Technology (Annex 3, point II.J.1) and have deepened this subject after hiring me as an assistant. At the time, I was intensively involved in the analysis of legislation regarding the registration of new substances under the REACH regulation. My task was to select the necessary physicochemical, toxicological, ecotoxicological and environmental properties for the manufacturing substance with a tonnage of 100 to 1000 Mg, in order to perform a chemical safety assessment for the Hydroxyester HE-1. The next step of my research was to evaluate the results of research and determine the impact of Hydroxyester HE-1 on the environment and human health. My long-term research in this subject have been described in detail in Chapter 4 of the Self-review.

The test results described above and other scientific studies related to the technology of manufacturing and application of the Hydroxyester HE-1 have been published in the following publications:

- Tic W.J., **Guziałowska J.**, 2009, The technology to manufacture environmentally friendly solvents based on oxo derived raw materials, The Prospects of Scientific and Economic Collaboration European Union and China in XXI Century. Environmental protection and technology, Oficyna Wydawnicza Politechniki Opolskiej, 373-381.
- Tic W.J., **Guziałowska J.,** 2009, Ekologiczne rozpuszczalniki farb i lakierów wodorozcieńczalnych - charakterystyka, własności fizykochemiczne i toksykologiczne, Zeszyty Naukowe Politechniki Opolskiej nr 331, Inżynieria środowiska. nr 331, 7, 21-30.
- Tic W.J., **Guziałowska-Tic J.,** 2010, Badania własności plastyfikujących produktów kondensacji aldehydu izomasłowego, Zeszyty Naukowe Politechniki Opolskiej nr 339, Inżynieria Środowiska, Red: Ulbrich Roman, 8, 27-41.
- Tic W.J., **Guziałowska-Tic J.**, 2011, Badania niezbędne do uzyskania certyfikatu substancji w systemie REACH, na przykładzie hydroksyestru HE1, Środowisko i Rozwój, 23(1), 65-77.
- **Guziałowska-Tic J.**, Tic W.J., 2011,Wymagania rejestracji produktów w systemie REACH na przykładzie Hydroksyestru HE1, Innowacyjne rozwiązania w przemyśle chemicznym, Red: Tic Wilhelm Jan, Oficyna Wydawnicza Politechniki Opolskiej, 7-18.
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In the following years, I used my knowledge of the chemical safety assessment by taking part in the research on the energy-ecological efficiency system for the combustion of liquid and solid fuels (Annex 3, point II.J.3). As part of this project, I took part in research on the synthesis of iron-based combustion modifier for liquid fuels. I also participated in studies on the effect of modifiers on the emission of pollutants into the atmosphere during the combustion tests of liquid and solid fuels. Because it is planned to produce an iron-based modifier in the amount from 100 Mg to 1000 Mg, as in the case of the Hydroxyester HE-1, I have analyzed the environmental impact of this environmentally friendly product. My long-term research in this subject have been described in detail in Chapter 4 of the Self-review. The test results described above and other scientific work in this field have been published in the following articles:

- Tic W.J., **Guziałowska-Tic J.**, 2011, Charakterystyka katalizatorów efektywnego spalania ciężkich olejów opałowych, Innowacyjne rozwiązania w przemyśle chemicznym, Red: Tic Wilhelm Jan, Oficyna Wydawnicza Politechniki Opolskiej, 55-66.
- **Guziałowska-Tic J.**, Tic W.J., 2012, Modifiers used in the combustion process of fuel oil and solid fuels, Chemik, 66(11), 1203-1210.
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- **Guziałowska-Tic J.**, Bok A., Tic W.J., 2013, Nowe rozwiązania proekologiczne spalania paliw, Chemik, 67(10), 881-888.
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- Bok A., **Guziałowska-Tic J.,** Wilhelm Jan Tic, 2014, Effects of catalysts on emissions of pollutants from combustion processes of liquid fuels, Civil and Environmental Engineering Reports,13(2), 5-17.
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- Tic W.J., **Guziałowska-Tic J.**, Junga R., 2015, The impact of catalytic additive for coal fuel on the environment emissions, Przemysł Chemiczny, 94(9), 1557-1559.
- **Guziałowska-Tic J.,** Tic W.J., 2015, The impact of an iron-based modifier for liquid fuels on human health and the environment, Proceedings of ECOpole, 9(1), 87-93.
- Tic W.J., **Guziałowska-Tic J.**, 2015, Aspekty ekologiczne i ekonomiczne stosowania modyfikatorów spalania paliw silnikowych, Logistyka, 4, 6216-6224.

After coming into the force of the Directive of the European Parliament and Council on the protection of animals used for scientific purposes and the requirements for reducing animal testing, I began to look for alternative methods to determine the impact of chemicals on the environment and human health. Based on the literature review, I decided that the best method would be a quantitative relationship between chemical structure and biological activity (QSAR methods). My long-term research in this subject have been described in detail in Chapter 4 of the Self-review. The results of these studies have also been described in two publications:

- **Guziałowska-Tic J.**, Tic W.J., 2016, QSAR methods as an alternative to animal testing in the threat assessment of toxicity and ecotoxicity of chemical substances, Przemysł Chemiczny, 95(8), 1475-1478.

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- Guziałowska-Tic J., 2016, Wykorzystanie metod QSAR do oceny wpływu substancji chemicznych na zdrowie człowieka oraz środowisko, Praca zbiorowa pod redakcją Wilhelma Jana Tica, Studia i Monografie z. 442, Politechnika Opolska, 119-133.

The use of oleochemical raw materials for the production of environmentally friendly products

In period 2011-2013 I actively participated in project on innovative technology of fat compounds treatment with the use of trigeneration (Annex 3, point II.J.2) for the company Magmar producing candles and grave candles. As part of this project, I worked on the analysis of environmentally friendly raw materials for the production of candles and grave candles, and their impact on the environment. The results of these studies have been described in three publications:

- **Guziałowska-Tic J.**, Hreczuch H., Tic W.J., 2012, Market search of oils and fats as raw materials for the oleochemical industry, Przemysł Chemiczny, 91(6), 1185-1190.
- Guziałowska-Tic J., 2013, Charakterystyka surowców do produkcji świec i zniczy oraz ich wpływ na środowisko, Chemik, 67(10), 1027-1034.
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An additional area of my scientific interest was also the possibility of using waste glycerine from biodiesel production. The results of these works have been described in two publications:

- **Guziałowska-Tic J.**, Tic W.J., 2011, Wykorzystanie odpadowej gliceryny z produkcji biodiesla, Kompostowanie i mechaniczno-biologiczne przetwarzanie odpadów, Red: Siemiątkowski G., Wydawnictwo Instytut Śląski, 155-163.
- **Guziałowska-Tic J.**, Tic W.J., 2012, Possible uses for glycerin - a byproduct of biodiesel production, VI Konferencja Ochrona i Inżynieria Środowiska – Zrównoważony Rozwój, Kraków.

Waste management and sewage sludge

In connection with the growing interest in waste-free technology, I worked on the subject of waste management and sewage sludge in the direction of their further use. I have been dealing with this subject since 2012. Currently, in close cooperation with West Technology & Trading Polska Sp. z o.o. I am the main contractor in the project: "Industrial research and development at WT & T Polska Sp. z o.o. in order to develop a comprehensive and effective technology for processing waste raw materials from wastewater treatment plants for the production of electricity, heat or cold with simultaneous total waste disposal", financed by the Opolskie Centrum Rozwoju Gospodarki, implemented from 2016 (Annex 3, Point II.J.5). The results of these works have been described in 4 publications:

- **Guziałowska-Tic J.,** Tic W.J., 2012, Zagospodarowanie komunalnych osadów ściekowych w województwie opolskim, Prace Instytutu Ceramiki i Materiałów Budowlanych, 5(10), 370-394.
- Guziałowska-Tic J., 2015, Removal of asbestos-containing materials of the example on the city Opole, Chemik, 10(69), 652-653.
- **Guziałowska-Tic J.,** Tic W.J., 2016, Ocena nowego systemu gospodarki odpadami w województwie opolskim, Praca zbiorowa pod redakcją Wilhelma Jana Tica, Studia i Monografie z. 442, Politechnika Opolska, 9-25.
- Tic W.J., **Guziałowska-Tic J.,** Pawlak-Kruczek H., Woźnikowski E., Zadrożny A., Niedźwiecki Ł., Wnukowski M., Krochmalny K., Czerep M., Ostrycharczyk M., Baranowski M., Zgóra J., Kowal M., 2018, Novel Concept of an Installation for Sustainable Thermal Utilization of Sewage Sludge, Energies, 11, 748.

Since 2010 I have been working closely with the industry. At that time, I participated in many 3-month and 6-month industrial internships, among others in the following companies: Mexeo, Magmar, West Technology & Trading Poland, Holpona, Inside, Inventia (Annex 3, point III.Q.2). The experience gained at that time has contributed to broadening my knowledge in many areas, such as environmental engineering, chemical technology, energy.

Since 2015 I have been working closely with West Technology & Trading Polska. I am currently the main contractor in a project funded by the National Center for Research and Development ppt. "Development of crystallization technology based on a new type of crystallizer for organic compounds from alloys in suspension", implemented since 2016 (Annex 3, point II.J.4).

6. Synthetic summary of scientific achievements

Before obtaining the doctoral degree, my output included 3 scientific publications. Since obtaining the doctoral degree in 2008, in which year I also started working as an assistant at the Faculty of Mechanical Engineering at the Opole University of Technology in the Department of Environmental Engineering, my scientific achievement have significantly increased. During this period, I published total of 35 publications (and 46 including publications in the cycle indicated as a scientific achievement), of which 6 (12) publications are in the Journal Citation Reports (JCR). Among publications other than those in the JCR database, after obtaining the doctoral degree I published 14 (17) articles and 10 chapters in monographs. I also published 2 (3) articles in JCR journal supplements, as well as 3 papers and conference summaries. I was a co-founder of two national and one European patent.

For publications from the period from obtaining a doctorate to the present, my total Impact Factor is 5,196 (18,456), Hirsch index according to the Web of Science - 2, while according to Google Scholar - 3. Total number of points calculated according to the MNiSW scoring and according to the year of publication is 306 (478). My publications were cited 6 times according to the Web of Science database plus one citation of the European patent in the Derwent Innovations Index and 10 times according to the Google Scholar database (without autocitation).

I regularly receive invitations to review articles in the field of engineering and environmental protection. In the period after obtaining the doctoral degree, I reviewed 5 articles in journals included in the JCR database, including the Journal of Cleaner Production (4) and Atmospheric Environment (1). In 2017, I made 2 reviews for the conference journal on Web of Science: E3SWeb of Conferences. In turn, since 2015 I have been a reviewer in the journal: Archive of Waste Management and Environmental Protection and since then I have made 9 reviews.

I actively participate in conferences, which confirms my participation in 24 international and national conferences (Annex 3, III.B). On all of them I had presentation or posters. Confirmation of my scientific activity are also awards for scientific activity (Annex 3, II.K), and invitations to scientific committees of international conferences (Annex 3, III.Q).

A detailed description of my academic achievements can be found in Appendix 3 to the Application, table 14 below is a synthetic statement.

7. Didactic, popularizing and organizational achievements

A detailed list of my didactic and popularizing achievements can be found in Chapter III of Annex 3 to the Application. Below I presented a synthetic description of the most important of my activities in this area.

As part of didactic duties resulting from working as an assistant, and since 2010 as an adjunct at the Department of Environmental Engineering at the Faculty of Mechanical Engineering of the Opole University of Technology, I have developed and implemented a number of subjects, primarily in the field of engineering and environmental protection, chemistry and environmental chemistry. I also take care of the chemistry laboratory, in which I conduct a number of laboratory classes in many fields of study of the Faculty of Mechanical Engineering, especially Environmental Engineering. Therefore, in 2015, I was the co-author of the script entitled "Laboratory exercises in general chemistry for fields of study at the Faculty of Mechanical Engineering". I also developed English-language courses for foreign students (ERASMUS). Since 2018 I have been conducting English-language courses at the Faculty of Mechanical Engineering of the Opole University of Technology: Mechanical Engineering BSc, Environmental Enginnering MSc (Advanced Technologies in Environmental Engineering). As part of these faculties, I have developed lectures, exercises and laboratory classes.

From the beginning as an adjunct, I actively participate in the academic care of graduates. Until now, I have been promoter of 19 Master's and 18 Bachelor theses. I am also involved in the system of quality assurance of education by being a syllabus coordinator in the field of Environmental Engineering.

In addition to the didactic and popularizing activities described above, I also undertake many organizational efforts for the Department, Faculty and University. I was member: of the faculty recruitment commission, faculty commission for educational programs. I am also active as a member of teams for educational programs in the following fields: Chemical and Process Engineering, Engineering and Apparatus of Industrial Processes, Power Engineering and Environmental Engineering. In the years 2014-2016, I was a member of the Faculty of

Mechanical Engineering planners. For the current term, I am a representative of the group of adjuncts in the Faculty Council.

Table 14. Synthetic summary of dr inż. Joanna Guziałowska-Tic scientific achievements (state by 13/11/2018)

List of achievements	Before the doctorate	After the doctorate	Summary
Total number of publications	3	46	49
The sum of points for publications according to the lists of Ministry of Science and Higher Education	8	306 (478)	314(486)
Total Impact Factor	-	18,456	18,456
Hirsch index according to the Web of Science	-	2	2
The number of citations according to the Web of Science	-	6 + 1**	6 + 1**
Publications in the Journal Citation Reports (JCR)	-	6 (12)	6 (12)
Articles in journals other than those in the JCR	1	14 (17)	15 (18)
Published abstracts and conference papers	-	3 (4)	3 (4)
Authorship in the monograph's chapter	2	10	12
Articles published in journal supplements	-	2 (3)	2 (3)
National and European patents	-	3	3
Participation in national research projects	-	5	5
Reviewing publications in journals from the JCR	-	5	5
Reviewing publications in magazines that do not have an Impact Factor (IF), listed in part B of the list of Ministry of Science and Higher Education	-	9	9
Participation in national conferences	5(6)*	16 (24)*	21(30)*
Participation in international conferences	5(8)*	8 (16)*	13 (24)*

()* - number of speeches in the form of papers or posters
( ) – publications included in the publication cycle
** - citation in the Derwent Innovations Index

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