Anna Makarova<sup>1</sup> Nataliya Tarasova Valery Meshalkin Igor Kukushkin Evgeniya Kudryavtseva Rafael Kantyukov Elena Reshetova

> Article info: Received 03.06.2017 Accepted 23.11.2017

UDC - 628.4.08 DOI - 10.18421/IJQR12.01-03

## ANALYSIS OF THE MANAGEMENT SYSTEM IN THE FIELD OF ENVIRONMENTAL PROTECTION OF RUSSIAN CHEMICAL COMPANIES

Abstract: Since 2007, many chemical industrial companies in the Russian Federation have been actively involved in the Responsible Care® international voluntary program. To implement this program, vast bodies of data on environmental impact assessments needs to be collected. This allows us to analyse the environment-oriented trends in economic and social activities, and to record the achievements and problems in this field. The collected large bodies of data are in many cases heterogeneous, since the report has been a voluntary initiative. To analyse the existing trends in business processes, authors applied the methodology for system analysis of large bodies of data and used their own heuristic approximation algorithm for the treatment of accumulated data. This algorithm gives us the unique possibility of evaluating the performance of both individual chemical companies in the framework of the Responsible Care® program and the Russian chemical industry as a whole.

*Keywords:* algorithm, environmental impact assessment, key indicators, the Responsible Care® program, chemical companies

## 1. Introduction

It is found that chemical companies had some responsibility for the increasing environment pollution (Meshalkin et al., 2004) and greenhouse gases emissions including  $CO_2$ , NOx, methane and fluoro hydrocarbons (Klemeš et al., 2016). The Responsible Care® voluntary international program (West, 2007) created in Canada in the 1980s (Simmons & Wynne, 1993) has been still widely used by chemical plants all over the world, at global (Lee et al., 2014)

and regional levels. The Responsible Care® program is positioned by many countries and organizations (APEC, 2011) as the main tool for self-regulation of environmental impact for chemical plants and as a voluntary tool for stimulating the continuous refinement of the main indicators in production processes, environment protection, health maintenance, assurance of safety and social responsibility (Bélanger et al., 2013). The program is aimed at the prevention of taking excessive normative regulatory measures by the state (Bélanger et al., 2009), and at the creation of a positive reputation in the community (Sandman, 2002). A study exists that shows that the probability of incidents decreases considerably in companies that are the

<sup>&</sup>lt;sup>1</sup> Corresponding author: Anna Makarova email: <u>annmakarova@mail.ru</u>



program members (Finger & Gamper-Rabindran, 2011). Some scientists have some doubts in the efficiency of the Responsible Care® program as a tool for minimising the impact of chemical plants on the environment (Gamper-Rabindran & Finger, 2013). A position exists that the main goal of the program may lie not in of the impact on minimisation the environment but in the manipulation of public opinions and resistance against the introduction of ecological regulation that is more economically onerous for companies (Givel, 2007).

From its start the program is favoured a considerable decrease in the environmental impact (Moffet et al., 2004). Various key performance indicators (KPI) are used for quantitative assessment of the efficiency of implementation of the Responsible Care® program, including in the field of environment protection from harmful impacts of chemical plants (ICCA, 2015). To date, large bodies of data on these KPIs have been collected for the period from 2000 until 2015 during the implementation of the Responsible Care® program. It should be noted that the use of indicators for the estimation of environmental impact assessment (Meshalkin et al., 2009) and sustainable development indicators (UN, 2014) is usual practice in the analysis of the state of complex systems (Klemeš, 2015). Some indicators are used for global assessments, such as the ecological footprints family (Čuček et al., 2012), and a chemical footprint (Tarasova and Makarova, 2016). It is proved to be difficult to assess the efficiency of implementation of the program in the field of environmental protection based on the collected indicators. For example, based on a system analysis of collected data, including those on the total chemical oxygen consumption (hereinafter, COC), emissions of SO<sub>2</sub> and NOx provided in the ICCA 2015 report, it was stated that it is impossible to compare these actual data quite objectively. The authors traced the trends and noted that the increase in the

number of reporting companies by more than 25% is accompanied by an increase in the emissions of nitrogen oxides (by no less than 25%) and a small COC increase.

The reliability of conclusions based on actual data decreases because of the gaps in the collected data. The gaps, i.e., empty arrays in these data, are due to the voluntariness of reporting by the plants, hence not all data for reporting periods were included in the aggregated industry report. Some one-time data were provided by various small- and medium-sized businesses that did not have a considerable effect on the aggregation of whole industry data. The companies that provided reports may have renovation, undergone opened new operations, been revamped, and/or enhanced their production capacities. This directly affects the reliability and amount of actual data presented in reports.

Since direct comparison of actual indicators may fail to give an unambiguous idea on the efficiency of implementation of the Responsible Care® program, we developed heuristic an original approximation algorithm for analyzing the key performance indicators of chemical companies-members of the Responsible Care® program in the field of environment protection obtained by interviewing chemical plants of the Russian Federation over a period of 10 y, which makes it possible to obtain refined estimates of the efficiency of the Responsible Care® program and perform a system analysis of various activities of the companies.

One of the tools for automatic monitoring of the abovementioned indicators and decisionmaking on minimizing of hazardous environmental impact of chemical plants, companies and supply chains of the chemical industry (Sarkissov et al., 2003), are automated systems of environmental controlling. The environmental controlling is management business process that а integrates following the processes: planning, accounting. analysis, standartization and control - into unified

system of accumulation, processing and compilation of information for making scientifically sound management decisions on minimization of hazardous impacts on the environment.

Controlling ensures the achievement of both short-term (operational controlling) and long-term (strategic controlling) goals stated basing on the indicators of environmental safety and resource efficiency of the chemical plant.

The main purpose of controlling is systemintegrated informational, analytical, instrumental and methodological support for decision-making in order to ensure long-term activity and sustainable development of the chemical plant. The main tasks of controlling are (Meshalkin et al., 2011):

- identification of the actual state of the plant as a whole and its subdivisions on the basis of monitoring of performance indicators (BSC-System) and KPI (for plants using the Responsible Care® program to monitor their activity);
- comparison of the achieved performance of the plant with the specified or scheduled ones (calculation of deviations) and identification of reasons for deviations;
- forecasting and planning of indicators of actual state and activity in future;
- maintaince of sustainable development of the plant and prevention of crises basing on definition of weaknesses and bottlenecks in the plant's activity (SWOT analysis);
- formation of arrays of information for making of rational management decisions to improve economic state of the plant (re-engineering of business processes and their optimization), including adoption of management solutions to ensure

environmental safety of chemical and technological systems and optimization of activity of the plant according to different criteria (ecological, technological, economic).

# 2. Development of the heuristic approximation algorithm

The subject of analysis consists of large bodies of data concerning the indicators of environmental impact assessment of in chemical companies the Russian Federation collected during a 10-y period. It should be noted that the Responsible Care® program is rather flexible (Fransen & Conzelmann, 2015), which allows one to adapt the program taking into account national specifics (Moffet et al., 2004) and results in certain differences in the number of indicators collected in various regions and countries. The data analysed in this paper are annual indicators (separately by companies) of impact on environmental subsystems:

- atmospheric air (amount of emissions of sulphur dioxide, volatile organic compounds, carbon and nitrogen oxides, methane and fluoro hydrocarbons expressed in t);
- water (chemical oxygen consumption, amount of waste waters and hazardous compounds discharged into water systems, including phosphorus and nitrogen compounds, expressed in t);
- solid wastes to be disposed (amount of toxic (classes I-IV) and nontoxic wastes (class V) expressed in t);
- indicators of energy and resource consumption;
- expenses on environment protection measures;
- production total.

At the end of 2015, over 60 Russian companies, including the largest Russian chemical companies: JSC «MChC Eurochem» and PJSC «SIBUR Holding»



(that are in the top hundred of the world largest chemical companies), PJSC «PhosAgro», JSC «United Chemical URALCHEM», PJSC Company «Nizhnekamskneftekhim». LLC «United Chemical Company Shchekinoazot» and many other, signed agreements on entry into the Responsible Care® program and provided reports. In total, the companies that have provided reports manufacture about one-third of all chemical products of the Russian Federation, which allows us, with a certain error, to extrapolate the obtained results to the entire chemical industry of the Russian Federation. The validity of this approach may be partially justified by the study (Lenox and Nash, 2003), according to which, the more significant a company's impact on the environment, the more it is inclined to join various ecological initiatives, such as the Responsible Care® program.

To perform the system analysis of estimates on the efficiency of environmental activities of chemical companies, authors used the original heuristic approximation algorithm. Its block diagram is presented in Figure 1.



Figure 1. Block diagram of the heuristic approximation algorithm for assessment of the efficiency of environmental activities of chemical companies

The main stages and steps of the heuristic approximation algorithm are as follows:

Stage 1. To estimate the environmental impact assessment of J Russian chemical companies and foreign companies in absolute terms:

- **1.1** to calculate the aggregated absolute indicators  $i_a{}^n$  (where *n* is the reporting year) of the environmental impact assessment of *J* chemical companies that provided reports  $(i_a{}^n = \sum_{j=1}^{J} i_j{}^n)$ ;
- **1.2** to determine the trends of  $i_a$  variation by years, using the linear approximation procedure and the least squares method;
- **1.3** to rank the countries by year *n* and by each indicator  $i_a{}^n$  by comparison of similar aggregated absolute indicators.

Stage 2. To estimate the environmental impact assessment of J Russian chemical companies and foreign companies in relatively specific terms (per volume of manufactured products in terms of monetary values and/or masses).

**2.1** to calculate normalized or specific (per volume of manufactured products; in mass terms  $V_m{}^n$  and/or in monetary terms  $V_s{}^n$ ) aggregated indicators  $i_{norm}{}^n$  (where *n* is the reporting year) environmental impact assessment of *J* chemical companies-members of the Responsible Care® program that provided the reports

 $i_{norm}^n = i_a^n / V_m^n$  and/or  $i_{norm}^n = i_a^n / V_s^n$ 

**2.2** to extrapolate the normalised aggregated indicators of the chemical industry of the Russian Federation in general  $i_{ind}$ <sup>n</sup>

 $i_{ind}^{n} = i_{norm}^{n} \times V_{m.ind}^{n}$  and/or  $i_{ind}^{n} = i_{norm}^{n} \times V_{3.ind}^{n}$ 

- 2.3 to determine the trends of i<sub>norm</sub> and i<sub>ind</sub> by single years using linear approximation procedures and the least squares method;
- **2.4** to compose the ratings of countries by separate year *n* and by each indicator  $i_{industry}^n$  by comparison of similar aggregated absolute indicators.

Stage 3. To estimate the efficiency of environmental activities of chemical companies-members of the Responsible Care® program.

3.1 to calculate the efficiency of

environmental activities by the i-th indicator  $E_j^i$  as the slope of the trend line of the indicator being estimated drawn on a set of complex plots for a particular company, for all *J* chemical companies that provided reports for more than 4 y;

- 3.2 to calculate the performance indicator for the branch of industry as a whole for the i-th parameter  $E_{mean}^{i}$  $(E_{mean}^{i} = \sum_{j=1}^{J} E_{j}^{j});$
- **3.3** to calculate the efficiency of environmental activity of chemical companies for 10 y  $E_{total}^{i}$  $(E_{total}^{i} = E_{mean}^{i} * 10/S$ , where S is

expenses of the chemical companies on environmental protection (alternatively, one can use  $S_{atm}$ , *i.e.*, expenses of chemical companies on atmospheric air protection).

It is proposed to approximate the results of performance calculation for 11 Russian chemical companies that provided reports in various periods by the indicator represented by the slope of the linear approximation trend line drawn on the set of complex plots as demonstrated in Figure 2.



Figure 2. Calculation of the efficiency of implementation of the Responsible Care® program by the «disposal of toxic wastes» indicator

\*The plots correspond to the disposal of hazardous wastes by separate chemical companies-members of the Responsible Care® program. Thin straight lines indicate the linear approximations determined for each company while



the dashed straight line indicates the resulting approximation for the industry as a whole

# **3.** System analysis of the results obtained in calculations

**System analysis of soil contamination estimates.** Soil contamination was estimated by the following indicators:

- the amount of hazardous wastes (hazard class 1-4) deposited by the companies;
- the amount of non-hazardous wastes (hazard class 5) deposited by the companies.

The results of calculated efficiency estimates of the deposited amounts of hazardous wastes by the chemical companies are shown in Figure 3.



**Figure 3.** Dynamics of hazardous waste disposal by years: a) for companies-members of the Responsible Care® program, the diagram is given for absolute indicators and for relative ones (per t of the product); b) for the entire industry

The system analysis identified an insignificant increase in the amounts of hazardous wastes disposed of by Russian chemical companies in the period from 2005 to 2007 and from 2008 to 2012 (Figure 3a). However, the specific amount of hazardous wastes per t of the products decreases continuously (Figure 3a), while recalculation

of the indicator for the chemical industry as a whole (Figure 3b) does not show considerable changes in the estimates of chemical waste disposal.

The results of estimations on the efficiency of chemical companies in the disposal of non-hazardous wastes are shown in Figure 4.



Figure 4. Dynamics of non-hazardous waste (hazard class V) disposal by years: a) for companiesmembers of the Responsible Care® program, the diagram is given for absolute indicators and for relative ones (per t of the product); b) for the entire industry

One can clearly see in the diagrams presented in Figure 4 that, though the

absolute amount of non-hazardous wastes disposed of by companies increases, the

specific disposal per t of the products decreased tenfold during the ten years of the program implementation, from 15 t/t to 1.65 t/t (Figure 4a). Extrapolation to the entire Russian chemical industry also shows decrease in the formation of non-hazardous wastes from 803 mln tpy in 2007 to 275 mln tpy in 2013 (Figure 4b).

We believe that it is inexpedient and noninformative to rate countries by this indicator, since, in accordance with the reporting terms, the countries used considerably differing national procedures to classify wastes by the degree of hazard.

The atmosphere pollution was estimated by a number of emissions of sulphur dioxide  $(SO_2)$ , nitrogen oxides  $(NO_x)$ , volatile organic compounds (VOC), and carbon monoxide (CO). The results of the system analysis of estimates of atmospheric emissions of the main pollutants calculated using the heuristic approximation algorithm are presented in Figure 5.





main indicators for companies-members of the Responsible Care® program; b) data normalised per t of the products; c) dynamics of variation in emissions for the entire chemical industry

Atmospheric emissions of sulphur dioxide and nitrogen oxides from Russian chemical companies-members of the Responsible Care® program increase in absolute numbers (Figure 5a) but decrease when recalculated to the produced amounts (Figure 5c). The absolute emissions of VOC decreased in 2008-2010 and then started to grow considerably (Figure 5a), but the specific VOC emissions per t of the products remained nearly constant since 2008 (Figure. 5c). Both the absolute and relative emissions of carbon monoxide increase abruptly (Figures 5a and 5c). In particular, this is due to the ever-increasing number of chemical companies that begin to monitor this parameter. Within the entire industry (Figure 5b), it can be concluded that emissions of  $SO_2$ , NOx and VOC remained nearly unchanged after 2008 (for sulphur and nitrogen dioxides, a minor decrease can be observed on comparison of the data for 2007



and 2013). The emissions of CO increased considerably. The Russian Chemists union that represents the chemical companiesmembers of the Responsible Care® program occupies positions 6-12 among the other associations that provide reports on SO<sub>2</sub> emissions and positions 4-8 on NO<sub>2</sub> emissions. In terms of VOC emissions, Russian companies are in most cases one of the three leaders, along with companies from France and Australia. The contribution of three countries in these greatest environmental pollution of VOC emissions.

The impact of chemical companies on climate change was estimated on the basis of emissions of greenhouse gases, including carbon dioxide. nitrogen oxide. hydrofluorocarbons, and methane. To make an overall estimate of the contribution of emissions of chemical companies to the greenhouse effect, the values were converted to CO<sub>2</sub> amounts. The conversion coefficients were taken from (Climate Change, 1995) for the average effect over 100 t/t. The calculation results obtained for the emissions of greenhouse gases converted to CO<sub>2</sub> amounts are presented in Figure 6.



**Figure 6.** Dynamics of emissions of greenhouse gases converted to CO<sub>2</sub> amounts: a) for companies-members of the Responsible Care® program, the diagram is given for absolute indicators and for relative ones (t/t of product); b) for the entire industry

The diagrams in Figure 6 demonstrate the dynamics of changes in emissions for the fast growing industry that is to a large extent analogous to the dynamics of wastes disposal, where the absolute amount of wastes increases but the amount per ton of the products decreases.

The estimation of the impact on water systems was performed using indicators such as COD, discharge of nitrogencontaining and phosphorus-containing chemical compounds, total amounts of discharged hazardous chemical compounds, amounts of consumed and discharged water. Estimation of the environmental impact assessment of chemical companies using the selected criteria expressed in absolute amounts does not reveal any clear dynamics (see Table 1). However, for all the indicators, a clear decrease in their specific values per ton or cost of the manufactured products is observed. A decrease in the environmental impact assessment of the entire chemical industry in terms of the selected indicators expressed in absolute amounts is clearly observed.

**Estimation of energy consumption.** Estimation of energy consumption by Russian companies has shown that this parameter has increased both in absolute and relative amounts from 2005 to 2013, but for the chemical industry as a whole, this figure decreases.

The results of system analysis of estimates on the environmental impact assessment of chemical companies obtained in this study are presented in Table 1.



	Analysis of changes in the indicator								
Indicator name	Absolute value	Per t of manufactured products	Per RBL of revenues obtained	In the entire industry					
Impact on soil									
Burial of toxic waste	Increased from 2005 to 2007 and from 2008 to 2013	Decrease	Decrease	Remains almost unchanged since 2008					
Burial of non- toxic waste	Increase	Decrease	Decrease	A decrease on comparison of 2007 and 2013 data					
	Imj	oact on atmospheric	air						
SO <sub>2</sub> emissions	Increase	Decrease	Decrease	An insignificant					
NO <sub>x</sub> emissions	Increase	Decrease	Decrease	decrease on comparison of 2007 and 2013 data					
Volatile organic compounds	A decrease from 2005 to 2008 and an increase from 2010 to 2013	A decrease from 2005 to 2008; no significant changes afterwards	A decrease from 2005 to 2010; no significant changes afterwards	No clear dynamics observed					
Carbon dioxide	Increase	Increase	Increase	Increase					
Greenhouse gases amounts converted to carbon dioxide amounts	Increase	Decrease	Decrease	No clear dynamics observed					
	Im	pact on water syste	ms						
COD	No clear dynamics observed	Decrease	Decrease	A clear decreasing dynamics					
Phosphorus- containing compounds	No clear dynamics observed	Decrease	Decrease	Decrease					
Nitrogen- containing compounds	An increase from 2005 to 2010 and a decrease from 2011 to 2014	Decrease	Decrease	Decrease					
Amount of hazardous compounds disposed of with effluent waters	No clear dynamics observed	Decrease	Decrease	A decrease until 2013					

**Table 1.** Results of the system analysis of the estimates on the environmental impact assessment of chemical companies-members of the Responsible Care® program



Table 2.	Results	of	the	system	analysis	of	the	estimates	on	the	environmental	impact
assessmen	nt of cher	nica	l coi	npanies-	members	of t	he R	Responsible	Ca	re® ]	program (contin	ued)

	Analysis of changes in the indicator						
Indicator name	Absolute value	Per t of manufactured products	Per RBL of revenues obtained	In the entire industry			
	Im	pact on water syste	ms				
Amount of effluent waters	An increase from 2005 to 2010; no clear dynamics is observed afterwards	Decrease	Decrease	Decrease			
Total water consumption	Increase	Decrease	Decrease	Decrease			
Power consumption							
Total power consumption	An increase from 2005 to 2013	An increase from 2005 to 2013	No clear dynamics observed	Decrease			

At stage 3 of the proposed heuristic approximation algorithm, we estimated the efficiency of chemical companies' activities based on the generalised individual achievements concerning the reduction of effluents, discharges and disposed wastes. The resulting efficiency estimates were aggregated and compared to the data on expenses on environmental protection (see Table 2).

Table 3.	Results	of the	system	analysis	of the	efficiency	of natur	e protection	activities	of
Russian c	chemical	compar	nies-mer	nbers of t	he Res	ponsible Ca	are® prog	gram		

Indicator name	Change in indicators	The decrease in environmental impact assessment in a 10-y period, kg/RUB			
		per RUB of environment protection	per RUB of atmospheric air protection expenditures		
		expenditures	r		
Impact on soil					
Burial of toxic waste	Increase	None	N/A		
Burial of non-toxic waste	Increase	None	N/A		
Impact on atmospheric air					
SO <sub>2</sub> emissions	Increase	none	N/A		
NO <sub>x</sub> emissions	Decrease	1.6*10 <sup>-3</sup>	1.1*10 <sup>-2</sup>		
Volatile organic compounds	Decrease	4.5	30.4		
Carbon monoxide	Increase	None	None		
Greenhouse gases	Increase	None	None		
Impact on water systems					
COD	Decrease	3.8*10 <sup>-3</sup>	N/A		
Phosphorus-containing compounds	Increase	None	N/A		
Nitrogen-containing compounds	Decrease	2.8*10-2	N/A		
Amount of hazardous compounds disposed of with effluent waters	Decrease	8.66	N/A		
Amount of effluent waters	Increase	None	N/A		

The first column of Table 2 provides results of calculation of estimates of changes in effluents, discharges and disposed wastes obtained by processing the annual reports from PJSC «Nizhnekamskneftekhim», JSC «Russian paints», LLC «United Chemical Company Shchekinoazot» and JSC «MChC Eurochem» for 9-11 years; CJSC «BASF» and PJSC «Khimprom» (Novocheboksarsk) for 6-8 years, OJSC ChC «Pigment», PJSC «SIBUR Holding», JSC «Polyef» and JSC «Caustic» (Volgograd) for 4-5 years; JSC «United Chemical Company URALCHEM», OJSC «Gazprom neftekhim Salavat», JSC «Sayanskkhimplast», OJSC «Stavrolen» and PJSC «PhosAgro» for three years. Together, these companies manufacture about 30% of chemical products in Russia, so the data obtained allow us to make predictive conclusions for the entire industry. The results obtained in the estimations of the efficiency of single companies (see Table 2) match the results obtained in stages 1 and 2 of the heuristic approximation algorithm, in estimation of aggregated indicators (see Table 1), from indicators of the dynamical of waste disposal, emissions of SO<sub>2</sub>, VOC, CO and greenhouse gases. However, the results obtained for nitrogen oxides showed positive rather than negative dynamics, unlike the aggregated absolute indicators. In the estimation of indicators of the hydrosphere

impact, the results only differ for phosphorus compounds: estimates on single companies give an increase in emissions (see Table 2), whereas the aggregated indicators show their decrease (see Table 1).

The last two columns (see Table 2) give calculations of the specific efficiency of activities (where a decrease was observed) in [kg/RUB of expenditures].

## 4. Automated systems of reporting and making decisions on minimization of environmental impact of the chemical industry

Environmental controlling informational systems (IS-EC) which is proposed for use by the companies solve such tasks such as monitoring. control. forecasting, optimization, management for purposes of hazardous industries and plants of supply chain of the chemical complex operated by automated control systems of technological (ACS-TP) and systems of processes industrial environmental monitoring. Each of the automated information systems collects a variety of information on technological and environmental parameters of the production process, basing on its goals and objectives (see Table 3).

Task	ACS-TP	AS-EM		
Monitoring of	Technological parameters	Environmental parameters		
Comparison of the parameters	To specified technological parameters	To MAC values		
Operation	Chemical and technological processes	Environmental safety		
Forecasting of Production quality		Environmental impact		
Prevention of emergency situations	Technological parameters beyond the specified ones	Excessive concentrations (over MAC)		
Optimization	By technological criteria	By environmental criteria		

**Table 4.** Comparison of tasks solved by ACS-TP and AS-EM

The following common tasks of the automated system of technological process control (ASC-TP) and the automated system of environmental monitoring (AS-EM) were

identified basing on the results of system analysis:

• collection, accumulation, storage and processing of large arrays of



technological and environmental information;

- information exchange with other logistics management systems;
- generation of array of input data for making science-based management decisions on optimization of industrial business processes.

The authors propose to create a centralized data storage as a single information resource (Figure 7), using large arrays of information from ASC-TP and AS-EM for environmental controlling tasks solution. The advantages of single information resource of ASC-TP and AS-EM as well as IS-EC are:

 information exchange with other information systems of logistics management of the company;

- availability of information . on technological parameters (input concentrations, veild final of products and wastes; volume of production, etc.) when constructing of mathematical models to predict environmental parameters (concentration of pollutants; discharges and emissions, etc.);
- using of information on environmental parameters (concentration pollutants; of discharges and emissions, etc.) for optimization of technological processes according to environmental criteria;
- obtaining of initial data for making decisions on optimization of technological processes according to economic criteria.





The methodology for development of complex of information models of large datasets used at all stages of data storage design: verbal, information-logical, relational and multidimensional data model is proposed.

Building of the mentioned complex of information models starts with a verbal model of the subject area (SA). The main source of information for IS-EM is the pollution control station (PCS) with controlmeasuring devices; equipment for

processing, storage and transmission of information, as well as control and life support systems. PCS can be located in stationary building (local PCS), as standalone facility (remote PCS) or as transportable version placed on any vehicle (mobile PCS). form – in the form of unstructured text, a set of separate statements, tabular or graphical form. Verbal model of PCS functioning processes, being the main source of environmental data, arriving at the storage data of IS-EM and IS-EC, is developed (Table 4).

Verbal SA model can be developed in any

No	Action
1	The control unit commands sensors to carry out measurement of the controlled
1.	parameters of pollution.
c	Sensors and gas analyzers produce electrical signals that correspond to value of the
Ζ.	controlled parameters.
2	AD converter of the data processing unit converts incoming analogous electrical signals
5.	into digital values of the controlled parameters.
4.	Actual values of the controlled parameters are placed into the local database.
5.	The control unit commands the data processing unit to calculate the average values.
6.	The data processing unit takes out the values for the last period from the local database.
7	The data processing unit averages out the collected values of pollution parameters and
7.	places them into the local database.
0	The control unit commands the data transfer unit to pass the results of the
δ.	measurements to the central control station.
0	The data transfer unit takes out the average values of the controlled parameters from the
7.	local database.
10.	The data transfer unit passes the average values to the central control station.

**Table 5.** Verbal model of pollution control process on PCS

The next step is formalization of the verbal model. It is made in a form of functional model PCS developed in accordance with the IDEF0 methodology. Context diagram of the functional logical-information model is realized as simulated system as «black box» (Figure 8).



Figure 8. Initial consolidated context diagram A-0 of functional logical and informational model of PCS



Detailed decomposition of the initial consolidated context diagram allows to develop the logical and information model of PCS business processes with the required level of detail. Figure 9 shows the decomposition of the first level of block A-0 context diagram.



Figure 9. Decomposition of the first level of A-0 functional logical and informational model of PCS business processes

The next step of the system analysis of business processes provides the transition from modeling of functions to simulation of large datasets flows. The model of datasets flows, in addition to external to the system entity objects displays the names of functions (phenomena, objects, processes), and abstract objects-storage (documents, databases, etc.). Data flow diagram DFD is shown in Figure 10.



Figure 10. Data flow diagram for PCS business processes



Basic entities (categories of similar objects) are «pollutant», «source of emissions», «control station» and «measuring equipment». In most cases, links between these entities are characterized as M:N («many-to-many») interactions. Next, the attributes to entities are set, and the overall model is normalized to eliminate data redundancy and functional dependencies between entities.

During the conceptual description of objects traditionally used model «Entity-Relationship» (Figure 11) in the form of ER-diagrams.



Figure 11. Fragment of data structure in model «Entity-Relationship» («ER-diagram»)

At the final stage of conceptual logical and informational design of data storage (Figure 12) the obtained model (in form of ERdiagram) is converted to relational data model. Then, basing on it one can build a multidimensional data model to enable data analysis using OLAP-technologies. The main dimensions of the multidimensional data model are time, production facilities, pollutants, sources of pollution and pollution control stations. Table representing the results of measurements of pollutants' concentrations are fact table.



Figure 12. Generalized structure of five-dimensional multidimensional data model in the form of a hypercube



JSC Nizhnekamskneftekhim the chemical company and leader in the implementation of the Responsible Care® program, was selected as an object of the study – object of environmental controlling. The following parameters were studied – climatic conditions in the controlled area, main directions of economic activity and related sources of pollution.

JSC Nizhnekamskneftekhim produces wide range of petrochemical products including monomers for synthetic rubbers, plastics, polystyrene, synthetic resins, solvents, surfactants, gaseous and liquid fuels, raw materials and other technical products.

There is a significant amount of pollutants both in main and auxiliary production lines. Major air pollutants are saturated and unsaturated hydrocarbons, benzene, isopropyl, ammonia, acetone, phenol, methanol, methylene chloride, isoprene, amylene and number of other substances (Table 5).

Name of	Limiting volue	Limiting	Hazard	Total emission	
substance	Linning value	value, mg/m <sup>3</sup>	class	g/s	ton/year
Aluminum oxide	luminum oxide MAC (average daily)		2	42.31	628,5
Tungsten oxide	MAC (average daily)	0.15	3	0.0002	0,00002
Titanium dioxide	ASLI	0.5	no	0.2	0,006
Iron oxide	MAC (average daily)	0.04	3	11.18	31.4
Potassium carbonate	MAC (one-time)	0.1	4	0.002	0,025
Potassium oxide (Quick lime)	ASLI	0.3	no	0.0013	0,007
Magnesium oxide	MAC (one-time)	0.4	3	0.0001	0.000008
Manganese and its compounds	MAC (one-time)	0.01	2	0.11	0,2
Copper oxide	MAC (average daily)	0.002	2	0.00003	0.0003
Sodium hydroxide	ASLI	0.01	no	0.4	4.7
Sodium carbonate	MAC (average daily)	0,15	3	0.019	0.46
Sodium sulfate	MAC (average daily)	0.3	3	0.00025	0.000004

**Table 6.** List of pollutants of the enterprise (fragment)

The regulations of IS-EM and its functioning in the framework of IS-EC was developed in order to ensure timely completion of data storage with reliable and actual environmental information. The IS-EM regulation defines the objects of control, location of control stations, parameters of control and frequency of control for purposes of environmental monitoring at JSC Nizhnekamskneftekhim and the city of Nizhnekamsk. Information on technological parameters of chemical-technological processes, emissions and wastewaters is passed to automated system of environmental monitoring. The results of measurements of pollutants' concentrations at stationary and mobile monitoring stations are placed into data storage of IS-EM and IS-EC and displayed in the software window at the control center.



As a result of the system analysis performed using the heuristic approximation algorithm that we developed, the following conclusions on the efficiency of activities of Russian chemical companies in the field of environment protection can be made:

- Basing on various environmental impact assessment indicators it is noted that the impact on environmental subsystems decreases. It should be noted that carbon dioxide emissions make an exception.
- 2) The waste management system should be distinguished as the top priority issue that requires close attention both from chemical companies and the government. The leading position of Russia in the amount of buried non-toxic wastes can be explained by the specifics of the Russian economics, but the waste management system needs to be developed in order to improve the position of our country in the world rating.
- The increase in atmospheric air 3) pollution by emissions of nitrogen, carbon and sulphur oxides is caused by the quickly increasing rates of production of chemical compounds. Despite this, system analysis has shown positive trends of the industry in decreasing the discharged amounts of chemical compounds that are most toxic for the organism. To a marked extent, this trend is favoured by the considerable increase in

expenditures for environmental protection.

- Decrease in the adverse effects of 4) chemical companies on water systems is primarily caused by the decrease in the amount of discharged waste water and implementation of closed water cycles. The system analysis that we performed allowed us to determine the types of activities for reduction of the total water consumption on a scientific basis. This reduction plays a critical role under the existing conditions of depletion of fresh water resources on the Earth and can lead to decrease of the amounts of phosphorus and nitrogen discharges.
- 5) The identified reduction of the total energy consumption by chemical companies due to the use of energysaving solutions as a result of systematic implementation of the Russian national energy-saving program can be considered as the best result of the Russian chemical industry that can be used to share Russia's experience with other countries participating in the Responsible Care® program.
- 6) In future, the developed heuristic approximation algorithm may be adapted for the system analysis of a large array of data on health protection and industrial safety provided by companies-members of the Responsible Care® program in their reports.

Acknowledgments: This research was supported by the Russian Science Foundation, grant 15-17-30016.

## **References:**

APEC, (2011). 2011/SOM3/CD/018. Strategic Framework for Chemicals in the Asia Pacific Region. *APEC Chemical Dialogue* September 13, 2011. Retrieved from http://mddb.apec.org/documents/2011/CDSG/CD/11\_cd\_018.pdf.



International Journal for Guality Research

- Bélanger, J., Topalovic, P., Krantzberg, G., & West, J. (2009). *Responsible Care: History & Development*. Retrieved from http://www.eng.mcmaster.ca/civil/facultypages/krantz11.pdf.
- Bélanger, J., Topalovic, P., & West, J. (2013). *Responsible Care. A Case Study.* Berlin, Boston: De Gruyter. Retrieved from http://www.degruyter.com/view/product/247600.
- Climate Change, (1995). *The Science of Climate Change: Summary for Policymakers and Technical Summary of the Working Group I Report*, 22. Retrieved from http://unfccc.int/ghg\_data/items/3825.php.
- Čuček, L., Klemeš, J. J., & Kravanja, Z. (2012). A review of footprint analysis tools for monitoring impacts on sustainability. *Journal of Cleaner Production*, 34, 9-20. doi: 10.1016/j.jclepro.2012.02.036
- Finger, S. R., & Gamper-Rabindran, S. (2011). Does industry self-regulation reduce accidents? Responsible Care in the chemical sector. SSRN Electronic Journal: November 2011. doi: 10.2139/ssrn.1990372
- Fransen, L., & Conzelmann, T. (2015). Fragmented or cohesive transnational private regulation of sustainability standards? A comparative study. *Regulation & Governance*, 9(3), 259-275. doi: 10.1111/rego.12055
- Gamper-Rabindran, S., & Finger, S. R. (2013). Does industry self-regulation reduce pollution? Responsible Care in the chemical industry. *Journal of Regulatory Economics*, 43, 1-30. doi: 10.1007/s11149-012-9197-0.
- Givel, M. (2007). Motivation of Chemical Industry Social Responsibility Through Responsible Care. *Health Policy*, *81*, 85-92. doi: http://dx.doi.org/10.1016/j.healthpol.2006.05.015
- ICCA, (2015). 2015 Responsible Care Status Report. Retrieved from https://www.icca-chem.org/wp-content/uploads/2015/09/2015-Responsible-Care-Status-Report.pdf.
- Klemeš, J. J. (2015). Assessing and measuring environmental impact and sustainability. Elsevier/Butterworth-Heinemann, Oxford. ISBN: 978-0-12-799968-5.
- Klemeš, J. J., Varbanov, P. S., Lam, H. L., & Yusup, S. (2016). Energy, Water and Environmental Footprint Interactions: Implications for the Major Economy Sectors of Europe, South East Asia and Worldwide. *Procedia Engineering*, 148, 1199-1205. doi: 10.1016/j.proeng.2016.06.630.
- Lee, K. E., Goh, C. T., & Mazlin, M. (2014). Initiatives and challenges of a chemical industries council in a developing country: The case of Malaysia. *Journal of Cleaner Production*, 86, 417-423. DOI: 10.1016/j.jclepro.2014.08.010/
- Lenox, M. J., & Nash, J. (2003). Industry Self-Regulation and Adverse Selection: A Comparison Across Four Trade Association Programs. *Business Strategy and Environment*, 12(6), 343-356. doi: 10.1002/bse.380
- Meshalkin, V. P., Klemes, J. J., Bulatov, I., Tsahalis, J., Shuvaev, V., Kapustenko, P., & Friedler, F. (2004). Recommendations on environmentally safe performance of a processing plant on the basis of analysis of pollution concentration distributions fields. *16-th International Congress of Chemical and Process Engineering «CHISA 2004»*, Prague, v.4.
- Meshalkin, V. P., Leontiev, L. I., & Butusov, O. B. (2009). A methodology for building the system of integral indices for assessment of the impact of metallurgical complexes on woodlands. *Chemist Engineer Encyclopedia*, *5*, 29-35.
- Meshalkin, V. P., Tokarev, A. L., & Ivanova, I. V. (2011). A methodology for organization of resources and energy controlling at the chemical enterprises using corporate instrumental informational systems. *Guide for business owner*, *12*,178-184.

- Moffet, J., Bregha, F., & Middelkoop, M. J. (2004). Responsible Care: A Case Study of a Voluntary Environmental Initiative. In K. Webb (Ed) Voluntary Codes: Private Governance, the Public Interest and Innovation, Ottawa: Carleton Research Unit for Innovation, Science and Environment, 177-208.
- Sandman, P. M. (2002). *Responsible Care* Been There. Done That. What's Next? Harvey Chartrand Interviews «Outrage Expert» Dr. Peter M. Sandman. Retrieved from http://www.psandman.com/articles/ccpa.htm.
- Sarkissov P., Meshalkin V., Zakhodyakin G., & Kapustenko P. A. (2003) Heuristic-numerical procedure for prediction of chemical plants emissions using logical-and-linguistic models. 53rd Canadian Chem. Eng. & PRES'03 Conf., Hamilton.
- Simmons, P., & Wynne, B. (1993). Responsible Care: Trust, credibility, and environmental management. In K. Fischer & J. Schott (Eds.), *Environmental strategies for industry: International perspectives on research needs and policy implications:* 201-226. Washington, DC: Island Press.
- Tarasova, N. P., & Makarova, A. S. (2016). Assessment of the Chemical Pollution in the context of the planetary boundaries. *Russian Chemical Bulletin, International Edition*, 65(5), 1-12.
- UN, (2014). United Nations Organization. Official site. Retrieved from http://www.un.org/ru/documents/decl\_conv/declarations/declarathenv.shtml.
- West, B. (2007). *Responsible Application of Chemistry: An Introduction to Responsible Care*. Retrieved from http://old.iupac.org/projects/2006/2006-047-1-022.html.



### Anna Makarova

Dmitry Mendeleev University of Chemical Technology of Russia, 125047, Moscow, Miusskaya sqr., 9 Russia <u>annmakarova@mail.ru</u>

## Igor Kukushkin

Dmitry Mendeleev University of Chemical Technology of Russia, 125047, Moscow, Miusskaya sqr., 9 Russia <u>ig.kukushkin@mail.ru</u>

### **Elena Reshetova**

Dmitry Mendeleev University of Chemical Technology of Russia, 125047, Moscow, Miusskaya sqr., 9 Russia reshetova lena@mail.ru

#### Nataliya Tarasova

Dmitry Mendeleev University of Chemical Technology of Russia, 125047, Moscow, Miusskaya sqr., 9 Russia <u>tarasnp@muctr.ru</u>

## Evgeniya Kudryavtseva

Ministry of Industry and Trade of the Russian Federation, 109074, Moscow, Kitaygorodskiy pr., 7 Russia evg73057932@yandex.ru

#### Valery Meshalkin

Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, 117901, Moscow, Leninskiy prosp., 31 Russia vpmeshalkin@gmail.com

### **Birhanu Beshah**

deputy Chief Engineer for Operation of Main Gas Pipelines of LLC Gazprom transgaz Kazan, 420073, Republic of Tatarstan, urban district of Kazan, Kazan, st. Adela Kutuya, 41 Russia glavgeo@mail.ru