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MODELLING THE RELATIONSHIP BETWEEN SELF-IGNITION TEMPERATURE AND PHYSICO-CHEMICAL PARAMETERS OF COAL MINE WASTE WITH THE APPLICATION OF THE PARTIAL LEAST SQUARES METHOD

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ABSTRACT

Purpose	The aim of the work presented in this paper was the construction of a regression model describing the relationship between the experimentally determined value of the maximum temperature observed during the coal mine waste fire and physico-chemical parameters characterizing the coal mine waste.
Methods	The model was constructed with the application of the Partial Least Squares method. The experimental data analysed was acquired through the use of a laboratory test stand with a fixed bed reactor and analytical method of gas chromatography.
Results	The constructed model was characterized by a good fit of the data used in its construction and the strong predictive ability for the new data. It illustrated the significant impact of the content of H and Fe ₂ O ₃ and trace elements: Co, Cu, Pb, Sr, V and Zn in a sample on the value of the maximum temperature reached during the fire of coal mine waste.
Practical implications	The practical importance of the work presented is clear in the light of the role of coal in the Polish economy and environmental aspects related to coal mining and the coal-based energy sector, in particularly to coal waste disposal and utilization. The model constructed contributes to the development of methods of self-ignition and fire risk assessment on coal waste dumps by determining the relationship between waste dump fire occurrence, the temperature observed during the fire and the physicochemical parameters characterizing the coal mine waste.
Originality/value	The novelty of the study presented in the paper consists in both finding the relationships modelled and the data extraction methods applied in the research field concerned.

Keywords

PLS, self-ignition, coal mine waste

1. INTRODUCTION

The increase in energy consumption and increased demand for fossil fuels have created new opportunities for the mining industry, especially in conditions of limited global resources of oil and natural gas (BP, 2013; Smoliński & Howaniec, 2010). The environment protection regulations, especially in terms of greenhouse gas emissions reduction, represent a major challenge for the coal mining sector and coal-based energy sector (Smoliński & Howaniec, 2007). Coal mine waste from the extraction and processing of coal poses a serious threat to the environment and human health. Areas of mine waste dumps are often characterized by high investment potential (Gogola, Bajerski, & Smoliński, 2012; Hudecek, Cerna, & Adamec, 2012; Kosmaty, 2011; Ostręga & Ubermann, 2010). Issues related to the protection of the environment include the quality of land, excessive content of

certain elements and compounds, leaching of pollutants that can migrate into the surface water and groundwater (POŚ, 2001; RMŚ, 2002) as well as the phenomenon of self-ignition of waste (Gogola, Iwaszenko, & Smoliński, 2012) and are of key importance in the management of these areas.

Mine waste dumps differ significantly in terms of waste composition. This results from the type of waste sources (one or several mines), the age of the dump and the differences in the operation of a mine (different technologies of coal processing). The oldest coal mine waste comes from the period when sorting stations operated in mines solely. Another type of waste is that from inactive slime separators. Slime has a specified market value: it is utilized in fuel blend production. However, self-ignition of slime stored in heaps often occurs during its extraction. Therefore, it is important to find the relationship between the waste dump fire, the temperature

observed during the fire and the physicochemical parameters characterizing the waste to estimate the risk of fire incidents in the areas where coal mine waste is stored. The construction of a mathematical model illustrating the relationship between the maximum temperature observed during the mine waste fire and physicochemical parameters characterizing the wastes was the subject of the work presented in the paper.

2. DESCRIPTION OF THE EXPERIMENTAL DATA AND THE METHOD OF THE PARTIAL LEAST SQUARES

Data characterizing the physical and chemical parameters, including the content of trace elements in samples of coal mine waste, for which self-ignition was observed, were organized in the matrix $\mathbf{X}(8 \times 31)$. The matrix rows describe waste samples, and its columns represent the physicochemical parameters tested (see Table 1), whereas the dependent variable $\mathbf{y}(8 \times 1)$ contains the maximum temperatures observed during the tests of self-ignition carried out in a fixed-bed reactor installation. The data organized in the matrix $\mathbf{X}(8 \times 31)$ were standardized since the physical and chemical parameters characterizing the examined waste were in different measurement ranges.

Table 1. The physicochemical parameters characterizing the coal mine waste samples tested

No.	Parameter	Unit
1	moisture content W^a	wt%
2	ash content A^a	wt%
3	content of volatile matter V^a	wt%
4	content of C	wt%
5	content of H	wt%
6	content of S	wt%
7	heat of combustion Q_s^a	kJ/kg
8	calorific value Q_i	kJ/kg
9	content of SiO_2	wt%
10	content of Al_2O_3	wt%
11	content of Fe_2O_3	wt%
12	content of CaO	wt%
13	content of MgO	wt%
14	content of Na_2O	wt%
15	content of K_2O	wt%
16	content of SO_3	wt%
17	content of TiO_2	wt%
18	content of P_2O_5	wt%
19	content of As	ppm
20	content of Ba	ppm
21	content of Co	ppm
22	content of Cr	ppm
23	content of Cu	ppm
24	content of Mn	ppm
25	content of Ni	ppm
26	content of Pb	ppm
27	content of Rb	ppm
28	content of Sn	ppm
29	content of Sr	ppm
30	content of V	ppm
31	content of Zn	ppm

2.1. Partial Least Squares Method

It is often necessary to match a linear function in order to find the relationship between the independent variables and the dependent variable or variables in studies conducted in the field of coal processing. For this purpose, the Linear Regression Method is applied and its generalization for the case when more than one parameter is measured, i.e. the method of Multivariate Linear Regression (MLR) (Brandt, 1998;

Martens & Naes, 1989; Mazerski 2000; Smoliński, 2012, 2014b). Data sets with correlated measured parameters are often found, which makes the application of the classical method of MLR impossible. In such cases, the method of the Principal Components Regression (PCR) (Joliffe, 1982; Martens & Naes, 1989; Smoliński, 2012, 2014b) or the Partial Least Squares (PLS) method (Djaković-Sekulić, Smolinski, Trišović & Uščumlić, 2012; Martens & Naes, 1987, 1989; Massart et al., 1997; Smoliński, Walczak & Einax, 2003; Smoliński, Zolotajkin, Ciba, Dydo, & Kluczka, 2009; Wold, 1981; Wold, Martens, & Wold, 1983) are most commonly used. The PLS method was applied in the study presented. In the PLS model, latent variables are established, which differ from the Principal Components applied in the PCR method. Namely, the principal components of the PCR method are constructed so as to maximize the description of the variation of the data, i.e., all the variables in block \mathbf{X} are taken into consideration, yet in the case of PLS models, latent variables are constructed in such a way as to maximize the description of the covariance between \mathbf{X} and \mathbf{y} .

The developed calibration models should not only be characterized by a good fit to the studied data, but especially by their strong prediction abilities for new objects. Cross Validation (CV) procedure was applied in order to determine the optimum complexity of the PLS model (Wold, 1978).

3. RESULTS AND DISCUSSION

An analysis of the physicochemical parameters for 12 coal mine waste materials collected from mine waste dumps located in the Silesian region has been presented (Smoliński, 2014a). The self-ignition temperature was determined experimentally for these samples (Gogola, Iwaszenko, & Smoliński, 2012). The self-ignition effect was observed for eight of them. Table 2 shows the maximum temperature values that were obtained under laboratory conditions during the test of self-ignition of 150 g waste in the fixed-bed reactor installation.

Table 2. The maximum temperature reported in tests of coal mine waste self-ignition in the fixed-bed reactor installation

Sample No.	Temperature, °C
1	434
2	292
3	364
4	275
5	251
6	293
7	360
8	462

A regression model was constructed, describing the relationship between the experimentally determined value of the maximum temperature observed during the fire of coal mine waste dumps, and physicochemical parameters characterizing waste samples. The maximum number of uncorrelated variables is indicated in the rank of a matrix, which is, by definition, equal to the smaller dimension of the matrix $\mathbf{X}(8 \times 31)$, in which physicochemical parameters characterizing the tested waste are arranged. In the case of data under consideration, the matrix rank is equal to eight. This means that the maximum number of uncorrelated parameters is eight. The parameters in the matrix analysed are correlated and it is not possible to construct a model describing the relationship

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