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Application of the Regression Function for the Description of Sorption Process

Abstract

The number of environmentally dangerous substances which the Fire Department has to face with, is increasing annually. Therefore, the aim of this study was to prepare a mathematical description of the sorption process.

The sorption process was performed in the laboratory scale. On the Petrie dish different sorbates with total amount of 100cm³ and exposed to different types of sorbents were analyzed. In this research the diesel oil and the petrol as well as sand and compact were analyzed. The time of sorption process and the changing weight of the sorbate were monitored. Next, the linear and non-linear regression was applied for the description of the sorption process.

It was presented that linear approach is not suitable to describe the results of the sorption process for dry sand and compact in the contact with Gasoline and Oil. In the first step of the sorption process a dynamic and prompt increase of the sorbate amount is observed, while at the end of the process the increase is more stable. Therefore, the non-linear regression mimics more accurately the shape of the experimental results compared to the linear approach.

Keywords: oil sorption, linear regression, non-linear regression

Zastosowanie regresji do opisu procesu sorpcji

Abstrakt

Liczba substancji niebezpiecznych dla środowiska, z którymi musi corocznie zmierzyć się straż pożarna rośnie. Z tego względu dokładne opisanie procesu sorpcji w warunkach laboratoryjnych pozwoli lepiej poznać właściwości sorbentów. Celem niniejszych badań było przygotowanie matematycznego opisu procesu sorpcji i ocena, który z modeli najlepiej opisuje dane uzyskane w laboratorium.

Proces sorpcji przeprowadzony był w skali laboratoryjnej. Na szalce Petriego analizowano różne sorbaty o całkowitej objętości wynoszącej 100 cm³ i poddawano działaniu różnego typu sorbentów. W niniejszym badaniu analizowano olej napędowy i benzynę, a także suchy piasek i sorbent compact. Wśród analizowanych parametrów były czas procesu sorpcji i zmiana masy sorbatu. Co więcej, do opisu wyników procesu sorpcji zastosowano regresję liniową i nieliniową.

Na podstawie otrzymanych wyników stwierdzono, iż regresja liniowa nie jest odpowiednia do opisu wyników procesu sorpcji dla suchego piasku i sorbentu compact w kontakcie z benzyną i olejem napędowym. Zarówno dla oleju napędowego jak i benzyny w kontakcie z suchym piaskiem i sorbentem compact w pierwszym etapie procesu sorpcji obserwowano dynamiczny i szybki wzrost objętości sorbatu, podczas gdy na końcu proces sorpcji stabilizował się. Z tego względu regresja nieliniowa odzwierciedlała dokładniej kształt wyników eksperymentalnych w porównaniu do regresji liniowej.

Słowa kluczowe: sorpcja oleju, liniowa regresja, nieliniowa regresja

1. Introduction

Due to the fact that substances considered as dangerous are practiced on a daily basis by the the majority of population, the activities of the Fire Department in the field of chemical and ecological protection are more and more demanding (Zuo-fuYu and Jia-linGuan, 2016). The basic duties of the Fire Department include i.e. protection against the environmental contamination by oil as a result of the vehicle collision (Lee and Jung, 2013; Papadonikolaki G. et al., 2014). Therefore, substances with the sorption properties, so-called the sorbents, which can occur in many forms, are able to collect not only the petroleum substances e.g. hydrocarbons, but also other dangerous substances, such as acids and alkalis (Demirel Bayik and Altin, 2017; Dong et al., 2016; Thinakaran et al., 2008). The most frequently sorbates, however limited in range, are oil spills which appear during the car accidents. In such situations, the activities of Fire Department are limited to stop the spreading of the dangerous substances, and bringing the road surface to its pre-event state (Ting Dong et al., 2015). Therefore, after the car accidents, the choice of the right sorbent based on its properties is not very important. However, in case of huge leakages e.g. on seas, selection of the proper type of sorbent is mandatory, while application of the material with the best sorption properties may limit at the costs of operations (Eakalak Khan et al., 2004). Therefore, the aim of the study was to compare different mathematical descriptions of the sorption process and to verify which model describes sorption process better.

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2. Material and Methods

In this research we proposed the mathematical description of the sorption process concerning two different types of sorbents. In the first step we prepared an experiment composed of the following substances: sorbates (100% of Gasoline, 100% of Oil and 50% of Gasoline and 50% of Oil) as well as two sorbents (dry sand and compact). Next, in the laboratory scale the sorbates were mixed on the Petrie dish. Each time the total amount of investigated liquid was equal to 100cm while the amount of the analyzed sorbent was equal to 50g. For the purpose of sorbate and sorbent contact an experimental set-up was prepared (Fig.1).



Fig. 1. Experimental setup, composed of: A – the Petri dish; B – an electronic weight; C – an anti-vibration table; D – a cylindrical container for analyzed sorbent; E – a telescope Source: authors

Each time analyzed sorbent was placed in the cylindrical container (Fig.1D), hanged on the telescope (Fig.1E) above the Petrie's dish (Fig.1A) and below the electric weight (Fig.1B), placed on the anti-vibration table (Fig.1C). In the research the sorbate weight every 10 s was acquired, until the same value appears for three times.

Next, attempts of mathematical description of the results of sorption process with a linear and non-linear regression was undertaken. For the comparison of both approaches following parameters were analyzed: R square, standard deviation and residuals. Moreover, graphical presentation of proposed regression was presented. Additionally, the residuals were calculated. If the model fits to the experimental data correctly, the residuals would approximate the random errors that make the relationship between the experimental and fitted values. While, if the non-random structure of the residuals appears it suggests that the model fits the data poorly.

3. Results

The results of the sorption process was presented as an amount of sorbate in function of time. It was observed that for dry sand in contact with Gasoline as well as Oil (Fig.2a) sorption was lower compared to compact in contact with the same sorbates (Fig.2b). Each time sorbate amount for the dry sand stopped at the level of approximately 8–11g. While, for the compact sorbent balance for the sorbate amount was achieved for approximately 18–20g.



Fig. 2. Experimental results of the sorbate amount in function of time for: a) dry sand as a sorbate, b) compact sorbate Source: authors

In the first stage of the sorption process a dynamic increase of the sorbate amount was noticed, approximately 200 s and 500 s for the dry sand and compact, respectively (Fig.3a–b).While, at the end of the sorption process stabile but relatively slow increase was observed (Fig.3b and Fig.3 c–d).



Fig. 3. Experimental results of the sorbate amount in function of time for: a) dry sand as a sorbate, b) compact sorbate Source: authors

First, the linear regression was applied for the description of the sorption results and the received results of the R square were extremely low (0.32 - 0.62) (Table 1). However, when the non-linear regression was used, the R square values for non-linear regression were higher compared to the linear one, and were in range of 0.50 – the R square values for compact in contact with Gasoline and Oil were higher compared to the application of sand for the same sorbates.

Each time for the linear regression the intercept coefficient "b" was expressed as a positive value as well as slope coefficient "a".

Analyzed case	Equation	R square
Sand Gasoline (100%)	f(x) = 0.0041x + 6.42	0.32
Sand Oil (100%)	f(x) = 0.0024x + 13.59	0.58
Compact Gasoline (100%)	f(x) = 0.0043x + 7.32	0.44
Compact Oil (100%)	f(x) = 0.0033x + 13.43	0.62
Sand Gasoline – Oil (50% – 50%)	f(x) = 0.0048x + 7.02	0.49
Compact Gasoline – Oil (50% – 50%)	f(x) = 0.0027x + 14.45	0.60

Table 1. Linear description of the analyzed sorbents and the sorbates fordifferent process conditions

Table 2. Non-linear description of analyzed sorbents and sorbates for
different process conditions

Analyzed case	Equation	R square
Sand Gasoline (100%)	$f(x) = -0.000022^2 x + 0.016x + 5.38$	0.50
Sand Oil (100%)	$f(x) = -0.000002^2 x + 0.007 x + 5.38$	0.63
Compact Gasoline (100%)	$f(x) = -0.000015^2 x + 0.015 x + 6.01$	0.74
Compact Oil (100%)	$f(x) = -0.000003^2 x + 0.010x + 11.03$	0.80
Sand Gasoline – Oil (50% – 50%)	$f(x) = -0.000017^2 x + 0.017 x + 5.49$	0.72
Compact Gasoline – Oil (50% – 50%)	$f(x) = -0.000002^2 x + 0.009 x + 11.89$	0.79

Moreover, the analysis of the standard deviation (SD) for the linear (0.97– 1.67) and non-linear (SD: 0.80–1.21) regressions indicated lower values of SD for the non-linear approach (Table 3). Additionally, SD values for the dry sand gave lower values when calculated with either the linear regression (SD: 0.97–1.40) or the non-linear regression (SD: 0.80–1.10).

Analyzed case	SD – linear equation	SD – non-linear equation
Sand Gasoline (100%)	0.97	0.84
Sand Oil (100%)	1.40	1.10
Compact Gasoline (100%)	1.06	0.86
Compact Oil (100%)	1.59	1.16
Sand Gasoline – Oil (50% – 50%)	1.08	0.80
Compact Gasoline – Oil (50% – 50%)	1.67	1.21

Table 3. Comparison of the standard deviation SD for the linear and non-lineardescription of the sorption process for different conditions

Graphical presentation of the regression method reflected that the non--linear approach much better mimics experimental results (Fig. 4a–f). Each time the application of the linear regression indicated the constant increase of the sorbate amount, which was contrary to the acquired results. While, the shape of function prepared with the non-linear regression mimics experimental results much better compared to the linear equation. The starting point for both, the linear and the non-linear regression, was a positive value, on the contrary to the acquired results. However, the difference between the experimental and numerical results was much lower for the non-linear regression compared to the linear regression. Depending on the analyzed case it was equal to 6.40-14.40 and 5.40-11.90 for the linear regression and the non-linear regression, respectively. Moreover, there was a difference between the numerical and experimental in the end points. Each time for the linear regression the end point was higher compared to the experimental result (approximately 6%), while for the non-linear regression lower values were observed (approximately 5%).

Moreover, the analysis of residuals indicated that in case of the non-linear regression they were distributed randomly. While, for the linear regression non-random structure of the residual was evident. Therefore, it suggests that the non-linear regression fits the data well, while the linear regression fits the data poorly.



Fig. 4. Experimental results of the sorbate amount in function of time for: a) Sand with 100% of Gasoline, b) Compact with 100% of Gasoline, c) Sand with 100% of Oil, d) Compact with 100% of Oil, e) Sand with Gasoline and Oil (50% – 50%), f) Compact with Gasoline and Oil (50% – 50%). The blue color – experimental results; grey color – the linear regression; orange color – the non-linear regression Source: authors

4. Conclusions

In this research it was presented that the linear approach is not suitable to describe the results of the sorption process for dry sand and the compact in contact with Gasoline and Oil. In the first step of the sorption a dynamic increase of the sorbate amount is observed, while at the end the process it is more stable. Therefore, the non-linear regression mimics much better the shape of the experimental results compared to the linear approach.

Moreover, for the linear and non-linear regression the starting point was a positive value, which was in opposition to the acquired results. However, the difference between the experimental and the numerical results was much lower for the non-linear regression, compared to the linear regression. Furthermore, there was a difference for the end points between the numerical and the experimental. Each time for the linear regression the end point was higher, compared to the experimental result (approximately 6%), while for the non-linear regression the lower values were observed (approximately 5%).

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