

## THE DEVELOPMENT OF SOFTWARE USING FOR PROCESSING DATA FROM THE LABORATORY SOIL VAPOUR EXTRACTION TEST

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**Abstract:** *SVE laboratory test is designed to find out if it is possible to take away pollutant on locality by use of soil vapour extraction (SVE). Main objectives of this work are to study the sorption mechanisms of volatile organic compounds on soils and to suggest a device with continual data gathering and optimal process of laboratory SVE test. The designed device was experimentally verified on soil samples with different elemental compositions. Practical benefit of this work should be simple functional software, which will process and evaluate measured data. Output will be idea of the best possible pollutant take away process.*

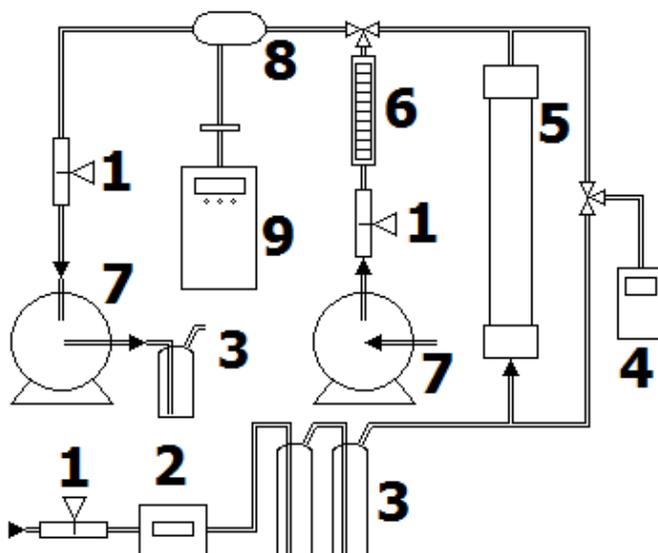
**Keywords:** volatile organic compound, soil vapour extraction, sorption, fugacity

### INTRODUCTION

Soil vapour extraction (SVE) uses vacuum pressure to remove volatile and some semi-volatile contaminants from the unsaturated zone of soil. The method is mainly used in the in-situ manner, seldom in ex-situ. It is aimed to reduce the concentrations of oil and chlorinated hydrocarbons present in soil. Laboratory SVE tests are carried out on a sample of soil directly from contaminated sites which is located in a steel sampling column. The air passes through the soil sample under laboratory conditions. It is monitoring of the development of concentrations in the air outgoing from the sample, flows and pressures in relation to time (fig. 1).

During extraction of volatile organic compounds (VOCs) from soils is gathered large amount of data from measuring devices, which must be correctly explained and are used to calculate and assess process of volatile organic compounds extraction from soils. Description and calculation of this process is very time consuming and can be burdened by mistakes. To avoid these mistakes and shorten time needed to calculations, made our team decision to create two computer programs. First program called “Venting” was programmed by Marek

Martinec and is used for evaluation and calculation in laboratory SVE tests and remedial procedures.



**Fig. 1.:** Scheme of experimental laboratory SVE device; 1 – flow controller, 2 – flow meter, 3 – washing apparatus, 4 – pressure measurer, 5 – sampler with soil, 6 – rotameter, 7 – pump, 8 – glass mouse, 9 – PID detector with filter

Second program called “Atmogeochem” was created by Veronika Rippelova and is able to calculate model of sorption from measured data. This program uses two sorption models. The literature describes equilibrium sorption either on natural organic matter or on clay mineral whose characterization is hindered by the use of non-uniform methods. First sorption model calculate only with the sorption on organic matter which is directly proportional to the mass content of the organic carbon (OC) measured by the organic elemental analysis.

Second sorption model presents a new way of calculations of partition coefficient  $K_d$  for VOCs in soils based on a new sorption model OC-Al-Si (Rippelova 2009). In new OC-Al-Si model, the priority for the sorption is attributed to organic matter and clay minerals. The sorption on organic matter is directly proportional to the mass content of the organic carbon. It is same like in the first sorption model. The sorption of VOCs on mineral component depends on the mass content of silicon and aluminum in the soil matrix. Silicon and aluminum content was measured by XRF. They appeared in soils mostly in clay minerals.

The designed model was experimentally verified in previous author's works with the help of the static headspace and extraction methods, recommended by US EPA (EPA method 5021A 2003). We examined the effects of the content of organic carbon, silicon, aluminum and moisture on the

sorption of VOCs. The OC-Al-Si model was compared with already-existing models that differed in  $K_d$  calculating. The comparison with simpler models showed that the OC-Al-Si model describes the sorbent properties of soil more accurately and with a higher recovery factor. The difference between estimated and measured values did not exceed 20 %.

## **METHODS**

First program called “Venting 1.0.0.0” was programmed by Marek Martinec in software development environment CodeGear™ Delphi® 2009 and is used for evaluation and calculation in laboratory SVE tests and remedial procedures. This program is also able to read measured data from two devices. These devices are PID (photo-ionization detector) MiniRae 2000 and mass flow meter Brooks.

The program “Atmogeochem” created by Ing. Veronika Rippelova converts the concentrations of VOCs in the gaseous phase to their concentrations in the solid phase of the soil. The conversion is based on the equilibrium fugacity model of the environment (Trapp et al. 1998; Mackay 1979). The program was formulated to enable the interpretation of the headspace method data and the interpretation of the data obtained by the atmogeochemical investigation. Application Lazarus was used as a programming environment for FreePascal Compiler.

## **RESULTS AND DISCUSSION**

All measured data are displayed and sorted into the chart placed in the left part of program window and all measured and calculated data are shown as a graph in the right part of program window. Graph displays minimal, average and maximum measured data from PID detector and all data are presented as mass concentration in  $\text{mg}\cdot\text{m}^{-3}$  sorted by SVE duration. Next is included time behaviour of temperature [ $^{\circ}\text{C}$ ] and air flow expressed as  $\text{l}\cdot\text{min}^{-1}$ . All calculated data are situated in the lower part of program window.

Program is simply controlled by using five buttons. These buttons are sorted in order of usage and named by their function. Successfully inserted data in each step are presented by green symbol displayed above button which belongs to propriate step. Unsuccessfully or missing data are presented as a red cross above button of propriate step. First step is used to enter interval of sampling adjusted on measuring devices. In second step is chart of compounds and their correction factors for each UV lamp of PID detector. In this step is possible to enter temperature which is used during calculations. If temperature is not set, the program will use average temperature measured by mass flow meter Brooks. Third step is used to load data files from supported measuring devices, first is loaded data file from mass flow meter Brooks and then is loaded

data file from PID detector MiniRae 2000.

When all measured data are loaded, program will calculate total time of SVE, total area under the curve displayed in the graph. This area is converted to total amount of extracted volatile contaminant by using total amount of flowed volume. Also are displayed maximum, average and minimum measured values from PID detector, average temperature and average air flow. Program also display chosen compound, UV lamp and correction factor, which were used to convert volume concentration to mass concentration. The next important calculated value is total amount of flowed volume. If we need to compare different runs of SVE, we can simply repeat first three steps of data entering and finally all runs will be displayed one after another in graph and calculation windows.

In any case if is need adjust or add new compounds and their correction factors, it is possible to change data file containing compounds and correction factors for each UV lamp of PID detector. Procedure of changing this file and path where to find this file is described in help window.

All measured data can be saved as a text file with default name "Data" followed by current date and time. Graph can be also saved as a bmp picture format with default name "Graf" followed by current date and time. Graph can be saved in full length or we can choose part of graph which will be saved. Graph allows us zoom in and zoom out displayed data, also is possible to switch on or off individual data series.

For help with using this program we can use at any time button called "Nápověda" placed in the upper right corner of main program window. In left part of help window is situated buttons, which contains help topics. After pushing buttons, help for chosen theme is shown in the right part of help window. Lower left corner of help window contains link to the support web page created for this program and email contact to author.

Button in main program window called "Sorpční model" is used to save data required for calculation of sorption model and opens program Atmogechem.

Atmogechem 1.0 allows the user to employ the basic input data pertaining to the contaminant and the soil and to calculate the sorption coefficient, the concentration of the contaminant in the solid phase, and its distribution among the individual components of the soil.

The soil input data can be processed in two ways. First if you enter the density of the soil particles and elemental composition, your output will be the conversion of  $\text{mg.m}^{-3}$  to  $\text{mg.kg}^{-1}$ . Second possibility is to add the porosity, moisture content and weight of the sample in a head-space vial. The outputs will expand of the distribution of VOCs in the soil environment. The program outputs are also important values of sorption coefficient and the fugacity, which can serve to calculate the concentrations of individual components of the soil environment.

## **CONCLUSION**

In practical result of this study are two compatible computer programs which can be used separately. These programs have wide application area in remediation technologies. Because the user of the program does not have to be an expert in environmental physical chemistry, the program *Atmogeochem* may find its place in the administrative area where it can be used to estimate the extent of soil contamination.

## **ACKNOWLEDGEMENT**

*This work was financial supported from specific university research MSMT no. 21/2010 and MSM 6046137308 of Ministry of Education, Youth and Sports of the Czech Republic.*

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