

The phenomenon of adsorption was discovered and described in 1771 by Scheele. In his studies, he observed that the charcoal has the ability to absorb certain gases, but only a little over 100 years ago, this phenomenon was for the first time mathematically described. One of the first mathematical models was proposed by Freundlich [1]. This model is based on dozens of experiments that the author carried out in the framework of his doctoral dissertation.

Another milestone in the description of adsorption phenomena was the work of Irving Langmuir in 1918 dedicated to the adsorption of gases on the surface of solids [2]. The results of these works were of great military importance, in the face of the ongoing World War I. In memory of all were fresh reports of the battle of Ypres (22 April 1915), where for the first time at the site of battlefield chemical weapon was used. So far unknown, deadly, barbaric weapons based on chlorine gas. It is known that chlorine gas is a gas highly caustic yellow inducing, mucosal edema, and tissue damage. Soldiers exposed to the gas, died in the terrible agonies, fighting for every breath.

As a result of these reports in laboratories around the world, scientists began investigations about ability to protect soldiers against chemical weapon. For effects we don't have to wait too long. Already in 1915 chemist Nikolai Zielinski (prof. University of St. Petersburg) developed the first mask based on the carbon filter. However, the principle of operation and efficiency of the mask, were not fully known. A significant milestone in this area the work of Irving Langmuir, who was engaged in quantitative description of adsorption phenomena on the interphase of gas-solid. It is worth noting that for these achievements he was awarded (Nobel prize in 1932).

The aim of the project is to confirm the proposed mathematical model of adsorption isotherm. This model based on the mathematical description of the kinetics of adsorption phenomena. As a result, formation of a general model which at the mathematical level, can either be brought back to the form of Langmuir or Freundlich isotherm.

To verify this model metal ions will be used. The choice is not accidental, since the physicochemical properties of most metals ions are well known and widely available in the literature. For determining the concentration of metal ions in aqueous solutions methods such as UV-VIS spectrometry, emission spectrometry MP-AES will be applied.

In all our experiments, commercially available activated carbons, in non-modified and modified forms are planned to be use. For this purpose, 2 different types of activated carbon will be chosen. Modification will be related to oxidation of activated carbon using modified Hummers method[22]. The second type of modification will be related to the reduction of oxygen containing functional groups by hydrogen at elevated temperature (350-500 °C). Results will be compared to find out if there is really strong relation between concentration of functional groups and the adsorption process.

New adsorption isotherm will be fitted to experimentally obtained data:

$$\frac{[A_{ads,x} \cdot C_{org,y}]_r}{[C]_{org,0}^y} = \frac{k_{1,obs}}{k_{2,obs}} \cdot [A]_{soln}^x$$

where:

$\frac{k_{1,obs}}{k_{2,obs}} = K$  equilibrium constant,  $[A_{ads,x} \cdot C_{org,y}]_r$  product – effect of adsorption of component A on functional

groups  $[C]_{org}$ ,  $[C]_{org,0}$  concentration of functional groups on the surface of activated carbon, x and y – an exponent factor related to the stoichiometry of the reaction.

The amount of the functional groups will be determined using Boehm methods.

As a final effect of the project, we expect to answer the question whether proposed adsorption isotherm is indeed the general description of the processes taking place on the surface of activated carbons. In such a case, determined equilibrium constant should be equal to the quotient of determined rate constants.

The amount of planned experiments is significant. Most experiments will be carried out by students of our Department. Obtained results will be used by them to write master's dissertation and BSc thesis. The academic staff will be responsible only for the supervision this work and final data processing.