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# QSAR MODELLING OF PREDICTING SOIL SORPTION COEFFICIENTS FOR ORGANIC CHEMICALS

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ABSTRACT

Adsorption of organic compounds on soil or sediment is the major factor determining their mobility, transport, and bioavailability in the Earth and aquatic environments. Organic matter is the immediate synthesis sphere in soil or sediment, and soil is primarily considered to be a separation process between soil organic materials and surrounding water. Soil adsorption coefficients normalized to sorbent organic carbon content (Koc) are currently used as quantitative measurements of adsorption of chemicals by soils, sediments from aqueous solutions. Soils have been recognized, generally, as the organic carbon content of the soil increases and the hydrophobicity of the chemical increases. As a result of this general observation, the organic carbon normalized sorption coefficient (KOC) was accepted as the unique properties or constants of organic chemicals. In sequence, KOC values are estimated by quantitative structure activity relationships (QSAR) developed by correlation with various physical or chemical properties and by structural details for the chemical hydrophobicity of octanol – water partition coefficients, aqueous solubility, molecular valency, such as Is related. Molecular weight, molecular surface area, and reverse-phase high-performance liquid chromatography retention time. The selection and application of the most applicable QSAR for the prediction of Koc depends on a number of factors, including the opportunity of required inputs, the suitability of the model to perform the chemical of interest, and the methodology for calculating the necessary topical or structural information. Any quantitative structures activity relationship (QSAR) model based on various physical or chemical properties and structural details have been developed and used to estimate the coke values of organic chemicals. Each QSAR modelling field is critically analysed and the advantages and / or limitations of different modelling approaches are given. The purpose of the paper is to study the QSAR for predicting log Koc vs. log Kow models, statistic modelling ,overview and evaluation of recent developments in molecular modelling.

## INTRODUCTION

QSAR models were built to estimate the soil sorption coefficients (log Koc) of substituted organic chemicals. quantitative structure–activity relationship (QSAR) modeling is a useful technique to correlate their physical, chemical, biological or environmental activities to their physicochemical property descriptors. Because the experimental determination is time-consuming and expensive, estimated values based on QSAR models are now widely used. Sabljic A et al. (1) were among the first researchers studying the applicability of molecular connectivity indices for the prediction of organic chemical's soil sorption coefficients. The purpose of this study was to systematically investigate the QSAR models of soil sorption coefficients for substituted organic compounds based on descriptors of n-octanol/water partition coefficients, molecular quantum chemical parameters, and molecular connectivity indices, respectively. Accurately (2)access human exposure to chemicals released into the environment and their adverse environmental effects, the environmental fate of chemicals must be known. Sorption of chemicals to soil/sediment is one

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of the major factors determining their mobility, transport and bioavailability in terrestrial and aquatic environments For various (3-5)chemical classes, organic matter (OM) is the primary constituent responsible for sorption in soil or sediment and sorption is considered as a partitioning process between soil OM and the surrounding water. This is of special relevance to the fate and behavior of pesticides, which are in continuous contact with soil particles following their application to the field. The soil(6) sorption coefficients are currently used as a quantitative measure of the extent of sorption of chemicals by soil/sediment from aqueous solutions They are defined as the ratios (denoted as Kd) between the concentrations of a given chemical sorbed by the soil and dissolved in soil water. In order to compare the soil sorption coefficients measured for different soils, the Kd values are often normalized either to the total organic carbon content of the soil (Koc) or the organic matter content of the soil (Kom). The soil sorption coefficients normalized to the soil organic carbon content (Koc)QSAR models based on a variety of physical or chemical properties and structural descriptors such as n-octanol/water partition coefficients, aqueous solubility, molecular connectivity indices, molecular weight, molecular surface area and reverse-phase high-performance liquid chromatography retention (3-5,7,8-13) Following the important topics of this research area, the log Koc versus log Kow model is seen in this chapter. the log Koc vs. log Kow models, Multilinear models(MLR), the models for ionized compounds and the major modeling efforts not covered by previous sections. Each of those subjects will be critically analyzed with a focus on more recent advancements and clear description of the advantages and limitations of different modeling approaches(14-15) In this case, specific recommendations are made on the application and reliability of specific QSAR models for estimation of soil coefficient coefficients of organic compounds. (16-18)in the adsorption of such solutes by soils from aqueous solutions because of the influence of this process on pesticide performance, mobility in the soil, and residue problems. Contamination of groundwater by pesticides and other agricultural chemicals by hazardous chemicals from waste disposal sites, and by gasoline and chemicals from underground storage tanks is becoming a major environmental problem. Although universal, this problem is particularly emphasized in the United States and other industrialized countries as well. prepared by the U.S. Environmental Protection Agency (19-21)and the Council on Environmental Quality indicate that up to 50,000 waste disposal sites in the United States may contain hazardous chemicals. Groundwater systems close to many of these sites are being slowly degraded, and the contamination often involves the presence of synthetic organic materials. arge sets of compounds.(22)The environmental fate of organic pollutants depends strongly on their distribution between different environmental compartments. The soil sorption coefficients are currently used as a quantitative measure of the adsorption of organic chemicals by soil from aqueous solutions. They are defined as the ratios between the concentrations of a given chemical sorbed by the soil and dissolved in soil water. In order to compare the soil sorption coefficients measured for different soils, they have to be normalized either to the total organic carbon content of the soil (Koc) In this paper, quantitative models for predicting soil sorption coefficients of organic chemicals will be described and evaluated. predicted and measured values of the soil sorption coefficients. The quality of the QSAR model confirmed the QSAR based on literature data, mandating the relevance of the data source.

**Factor Affecting**

The experimental determination of sorption coefficients such as the solid to solution ratio equilibration time, and phase separation technique can be important. Sorption generally decreases with increasing temperature. The impact of pH on the sorption of neutral organics is small; however, for ionizable organic chemicals, sorption coefficients can be greatly affected, because pH affects not only the speciation but also the surface characteristics of natural sorbents. The sorption of acidic compounds increases with decreasing pH,. Generalizations regarding the role of dissolved organic matter are more difficult to make, but the presence of dissolved organic matter has usually been observed to decrease the sorption, with the effect being greater for more hydrophobic compounds. Nonionic and anionic surfactants that increase the aqueous solubility of hydrophobic organics decrease sorption, whereas cationic surfactants that bind to negatively charged soil have been used to enhance sorption . However, observations of competitive sorption also have been reported and are thought to be the result of site specific sorption occurring in soil organic matter [23,24,25].A more detailed literature review of the factors potentially impacting sorption can be found in the recent article by dell Site [26]. Loss of compound by sorption onto the walls of the equilibration vessels, volatilization, and chemical or biological degradation also can affect the experimental determination of sorption coefficients. These potential loss mechanisms must be eliminated or accounted for if accurate sorption coefficients are to be determined. Although it is preferable to measure the concentration of the chemical in both phases and determine the mass balance to quantify potential loss mechanisms, this is not commonly done because of the increased analytical costs. Singh et al. [27] found that sorption coefficients obtained by measuring only the concentration in the solution phase were consistently higher than with those generated by using a mass balance approach when the concentrations in both phases are measured. A part of this overall objective, the present research developed QSAR to predict the adsorption of organic chemicals on activated Carbon without much more experimental data. The QSAR are based on isotherm data found in the literature. To develop QSAR for estimating adsorption easily in the water treatment industry, we established the following goals:-

1.Include as many and as wide a range of chemicals as possible. This necessitated using data from multiple sources.

2.Use a definition of absorbability that affects adsorption at low adsorbate concentrations.

QSAR stands for Quantitative structure Activity Relationship which offers the possibility for screening a large number of chemicals in short time and low cost. Using QSAR, we can obtain an activity of a chemical from its molecular structure only through studying a series of molecules of different structure and different observed properties and attempting to find relationships between structures and activity. It is usually applied to methods which correlate molecular structure to some kind of property (i.e. Physical, Biological, and Chemical). QSAR analysis is related not only the quality of input data but also the power of statistics. An important part of QSAR modeling is the use of software to create structure calculates descriptors and builds predictive models. DRAGON, MOPAC, Hyper chem., molecular modeling pro. etc. are kind of software through which structure of a molecule can be found and their properties can also be known e.g. structure of a molecule like Benzene, Phenols etc. and their physical or chemical properties such as solubility, boiling point, octanol/water partition, Molar Refractivity, Molecular Weight etc. can be available through software. QSAR was first developed by Hansh and Fujita 40 years ago for the development of QSAR requires three basic things.

1.An activity or property data set measured experimentally.

2.Molecular descriptors which are the Quantitative description of molecular properties.

3.Statistical techniques to establish the relation between molecular descriptors and activities.

## Modelling

### Statistical Modelling Process

There are five major [28]stages in the process of statistical modelling such as identification, fitting and estimation, validation, application, and iteration. Identification is the process of finding or choosing an appropriate model for a particular situation. There are no rigorous procedures that guarantee success. Systematically, there are two extreme approaches in the identification process: one which seeks a model on the basis of a rational argument from some knowledge of the real life situation without reference to any actual data (conceptual identification), and the other that considers only the data and their properties (empirical identification). In practice, both approaches should be used and combined to create the best models possible. Model fitting is the stage when we move from the general form to the specific numerical form, whereas the estimation stage represents the process of assigning numerical values to parameters in that model. The most frequently

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used and the best known method for the purpose of statistical modelling is least squares fit. The process of comparing the model with the observed world is called "validation." What is valid at one stage of a study need not be valid at a more developed stage. A model can be valid for one purpose, but not for another. The object of validation is to examine whether the model is a good (not true) description of reality in terms of its behavior and of its intended application(s). For logical reasons and convenience of presentation, the application is described as the last stage of the modeling process. However, in practice, the application must be a part of the very first consideration and taken into account when carrying out the processes of identification, estimation, and validation, since models are developed to help solve problems. If we ignore application during the modeling process, we might end up with an excellent model that will not solve our problem. Figure 1 gives a realistic view of statistical modeling being an iterative process. It is a process of continuous development, going back a stage or two to use additional information. The model is never "the model," final and unaltered. It is always a tentative model, which we shall use until we can improve it. We should always remember that in statistical modeling we are dealing with probabilities, distributions, populations, and uncertainties. One of the major sources of uncertainty is our data. When seeking to fit models to our data, we often find that an accurate fit requires more data than we can either practically or financially obtain. Even when we have enough data, we find that its quality is often far from perfect. We may have accurate data on some variables, whereas those for other variables may be inadequate. Very often, in order to have enough data, we are forced to collect data from various sources. The reliability and quality of such data will vary greatly. The limitations on the amount and quality of the data available reduce the precision with which we can fit and use the models.

## (QSAR) Models

Mathematical models that relate some chemical, biological, or environmental activity of interest to some quantitative structural descriptor or physico-chemical property are collectively known as quantitative structure-activity relationships (QSAR) models. QSAR models are usually developed for a group(s) of structural congeners. The primary objective in creating them is to predict the activities of untested congeners. The investigators also hope to understand better the mechanisms of action of structures under study. The statistical procedure used to derive QSAR models is the linear regression analysis, and it can be either single or multivariable, depending on the number of structural descriptors used in the particular analysis. The usual procedure in deriving QSAR models is stepwise and begins with the single variable regressions going from the simplest to the more complex structural descriptors. The next step is to screen multivariable models of increased complexity until the simplest model predicting activity of interest within the experimental error is found. Naturally, this stepwise procedure can be discontinued with the single variable models. To test the quality and accuracy of derived models, the following statistical parameters should be used: the single (r) and multiple (R) correlation coefficients, the standard error of the estimate (s), a test of null-hypothesis (F test), and the amount of explained variance (EV). A general statistical QSAR model for estimating soil sorption coefficients will be described due to its wide applicability domain and its extensive evaluation and validation procedure .Regression analysis is commonly based on a partial least squares projection, which is a multivariate statistical method; The key advantage of the QSAR model is that a known equation or the exact pathway of reactions is not necessary. A good QSAR model can rely solely on the structural and derived experimental characteristics of the targeted compounds to predict their activity. Additionally, unknown mechanisms could ultimately be disclosed through the analysis of how substituents impact QSAR correlations. Within the development of a QSAR, diverse parameterization is essential. Having a robust set of carefully chosen parameters increases the probability of unlocking a description of the mechanisms involved in a system. Three key components of a QSAR are: hydrophobic, electronic, and steric factors (29Hansch and Fujita 1995). various hydrophobic, electronic, steric and chemical properties that are commonly used in QSAR analysis.

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While diverse parameterization is essential to a QSAR, the selection of these parameters is crucial for the healthy development of the QSAR. A primary weakness in QSAR construction is often the selection of the parameters (Hansch and Fujita 1995). Poor parameter selection can lead to collinearity problems (i.e., when two parameters are directly affected by each other) thus creating false indications of correlation. Also, it is essential that parameters cover a wide range of space—i.e., the compound training set should be carefully selected so that multiple spectrums of the parameter scale are represented. This idea will be more fully developed in the Methods section with the introduction of Craig plots.Example of Parameters Commonly Used in QSAR Development. Hydrophobic Properties Π, LOG KOW Electronic Properties σInd, Resonance, Field Effects Steric Properties Molar Refractivity, Molal Refraction, Es Chemical/Physical Properties Boiling Point, Melting Point, Density, Molecular Weight, Aqueous Solubility, Enthalpy, Vapor Pressure Where σInd represents inductive effects described by the Hammett Constant and Es represents Taft’s steric factor. An important aspect of QSAR development that should be addressed is the selection of the training set and the specific parameters that are chosen for the correlations. There the literature, the first approach, developed by Hansch, is an approach favored by chemists in which the components within the QSAR are intellectually analyzed with respect to their chemical activity (Hansch and Fujita 1995). The second approach, described by Wold and Dunn (30 1983), is based on the statistical analysis of the components for QSAR development. Certainly, while the statistical method can prove to be insightful in some instances, a strong QSAR should be constructed with a vast understanding of the components in the system in order to avoid complications such as parameter collinearity, uneven spread of parameters, and the application of implausible mechanisms. In addition, it is also 26 important to consider the functionality of the compounds that are within the training set; only structural changes in functional groups that can be accurately represented by available parameters should be selected (Hansch and Fujita 1995). This present work approaches QSAR development for the adsorption process in three improved ways in comparison to past studies: 1. Dependent variables used are not from the literature, but were derived experimentally within this study 2. Degree of statistical analyses performed 3. Robust spread of parameterization empirically derived isotherm constants selected haphazardly from the literature can be detrimental to a study. The electronic, steric, hydrophobic, and chemical parameters used within this study were not experimentally derived within the scope of this work, yet each of these parameters has been well documented within the scientific community and has strict procedures for their procurement. However, in the case of deriving the isotherm constants, many variables are present: the type of carbon used, how it was activated, the conditions under which the carbon was kept, how it was added to the system, the pH of the water in the system, the solutes used within the system, the definition of equilibrium for that system, the concentrations of carbon and solute that were used, etc. In order to normalize these variables, each of the isotherm constants used within this system was derived under uniform experimental conditions. In order to measure the quality of the QSAR correlations, several statistical methods were used: R2 , adjusted R2 , standard error, F-Ratio, as well as Q2 (a tool that measures the predictability of a correlation). the study of Brasquet and coworkers (31]1997) refers to R2 values, but offers no other statistical validation for their resulting correlation. As was mentioned previously, the spread of parameters is an important concept in the selection of the training set. For this study, compounds demonstrating a wide range of steric, electronic, hydrophobic, and chemical properties were selected. This variety of parameterization is essential to aid in the identification of mechanisms involved in the are two basic approaches to QSAR that are seen in the Correlation.

## Molecular connectivity indices

Another widely used approach for predicting KOC, especially when experimental values of KOW or S are unavailable, is to employ QSARs developed with MCIs [32-36]. Molecular connectivity is a method of bond counting from which topological indexes can be derived from chemical structures. For a given molecular structure, several types and orders of MCIs can be calculated. Information on the molecular size, branching, cyclization, unsaturation, and heteroatom content of a molecule is encoded in these various indices . One significant advantage of using MCI–KOC regression models over property–KOC regression models is that once the model has been developed only the structure of the chemical of interest is required as input and no additional experimental parameters are needed. A detailed discussion of molecular connectivity and its application can be found in Kier and Kier and Hall [37].

**Estimation of KOC**

With the quantity of organic carbon used as the key sorbent characteristic describing the sorption of organic chemicals to environmental solids, most of the chemical descriptors (i.e., physical and chemical properties or structural descriptors) used in developing methods to estimate sorption coefficients have been related to hydrophobicity. Many of the reported quantitative structure–activity relationships (QSARs) for predicting KOC are based on the relationship between KOC and the octanol– water partition coefficient (KOW) or aqueous solubility (S)values as determined by regression analysis. These regression models are usually expressed by relating log KOC to log KOW or log S.Numerous estimation methods based on correlations with structurally derived parameters such as molecular connectivity indices (MCIs)[32-34,38-39] molecular surface area[40-42] the Multi linear relationships (MLRs) also have been reported. These correlations are especially valuable Molecular connectivity index based methods probably are the most widely used of the structural-based methods. Methods that use both MCIs and correction factors based on specific functonal groups also has been reported[38,39] which appears to extend the applicability of MCI-based estimation methods to a wider variety of compounds. The selection and application of the most appropriate QSAR for predicting $K_{OC}$ depends on several factors, including the availability of required input, the appropriateness of the model to the chemical of interest, and the methodology for calculating the necessary topological or structural information. Although the so-called $K_{OC}$ approach for estimating sorption coefficients is most appropriate for neutral, hydrophobic organic chemicals on environmental solids containing a significant amount of organic matter, this approach has been applied to a wide variety of chemical and soil types. The main reason for the wide acceptance of this approach is that it works reasonably well for a large number of organic chemicals and the organic carbon content of the environmental solid usually is available. In addition, an estimate of hydrophobic sorption or partitioning based on KOC often represents a minimum value or conservative estimate for the sorption of a particular hydrophobic organic compound. If specific sorbate–sorbent interactions also are involved, additional sorption may occur[44].Generally, other sorbent properties such as the type and amount of clay, soil pH, and hydrous oxide content have less effect on the sorption process except in situations where the organic carbon content of the sorbent is low or when the clay content is high . However, these correlations typically are valid only for specific soil–sorbent combinations and are considered far less general in their application. In addition, soil properties such as surface area directly related to the amount of organic carbon The remainder of this paper will focus on the use, applicability, and limitations of methods used to estimate KOC. A critical evaluation of the statistical validity of each method described in the following sections was beyond the scope of this review. In many instances, especially for the earlier estimation methods, little statistical information was presented. However, an attempt was made to provide the reader with some indication of model validity by listing the equation, the number of chemicals used to develop the model (n), and the coefficient of determination (r2) or correlation coefficient (r), if provided in the original reference. Before using any of the estimation methods described below, the reader is strongly encouraged to review the original citation. The reader also is encouraged to examine several previous reviews of sorption estimation techniques.[45-47]

Table 1. Representative examples of regression models used to estimate log organic carbon–normalized sorption coefficient (log KOC) from log octanol–water partition coefficient (log KOW)

| Equation | n | r2 | Chemical classes | References |
|---|---|---|---|---|
| Log KOC= 5 0.903 log KOW 1 0.0 | 72 | 0.91 | Wide variety | 50 |
| Log KOC= 5 0.679 log KOW 1 0.663 | 419 | 0.831 | Wide variety | 51 |
| Log KOC 5 0.544 log KOW 1 1.377 | 45 | 0.74 | Variety, mostly pesticides | 52 |
| Log KOC= 5 0.81 log KOW 1 0.10 | 81 | 0.887 | Hydrophobics | 46 |
| Log KOC= 5 0.52 log KOW 1 1.02 | 390 | 0.631 | Nonhydrophobics | 46 |
| Log KOC =5 1.03 log KOW 2 0.61 | 117 | 0.95 | Wide variety | 53 |
| Log KOC =5 0.63 log KOW 1 0.90 | 54 | 0.865 | Substituted phenols, anilines, and nitrobenzenes, chlorinated benzonitriles | 46 |
| Log KOC =5 0.47 log KOW 1 1.09 | 216 | 0.681 | Agricultural chemicals: acetamilides, carbamates, esters, phenylureas, phosphates, triazines, triazoles, and uracils | 46 |
| Log KOC= 5 0.545 log KOW 1 0.943 | 57 | 0.731 | Ureas | 51 |
| Log KOC= 5 0.433 log KOW 1 0.919 | 39 | 0.863 | Carbamates | 51 |
| Log KOC 5 0.402 log KOW 1 1.071 | 15 | 0.69 | Pesticides | 54 |
| Log KOC= 5 0.904 log KOW 2 0.539 | 12 | 0.99 | PAHs, chlorinated hydrocarbons | 55 |
| Log KOC =5 0.937 log KOW 2 0.006 | 9 | 0.95 | Triazines | 56 |
| Log KOC= 5 1.029 log KOW 2 0.18 Chlorinated hydrocarbons, pesti | 13 | 0.94 | Chlorinated hydrocarbons, pesticides | 57 |
| Log KOC =5 1.00 log KOW 2 0.21 | 10 | 1.00 | PAHs, aromatic | 58 |

## Summery and Conclusion

Estimating sorption with the KOC approach currently is the most widely used and generally applicable method for predicting the sorption of organic compounds to soils and sediments. For organic acids and bases, the KOC approach can still be applied if neutral form of the compound dominates at the pH of the soil solution. If both neutral and ionized forms of the chemical are present in significant quantities, the extent of sorption will depend on the fraction of each form present .As previously discussed, the two approaches considered to be the most generally appropriate for estimating KOC are

QSARs developed with log KOW and QSARs developed with MCIs. From the table no.1 it is clear that A review Representative examples of regression models used to estimate log organic carbon–normalized sorption coefficient (log KOC) from log octanol–water partition coefficient (log KOW)of the existing QSARs for predicting using the approach to estimate sorption coefficients will be presented. Other approaches may work well for specific classes of compounds . The addition of group contribution factors, as documented by Meylan et al. [48] generally improve MCI–KOC correlations for chemicals containing polar functional groups and should be used. For organic acids and bases, the method outlined by Bintein and Devillers [49] is the most well defined. However, given the well-documented variability inherent with experimental KOC values and the nonuniformity in the KOC data sets used to develop the estimation techniques, it must be emphasized that it is very difficult to evaluate the true accuracy of any of the models described in this review. It is also likely that many of the models reviewed here are overfitted and may give the user a false sense of accuracy. Until the variables impacting sorption are better quantified, truly accurate site-specific values of KOC are best obtained experimentally. The most appropriate use of KOC estimation methods is to provide a relative ranking of the tendency of an organic compound to sorb to soil or other environmental solid.

**Future Developments sorption coefficients Koc& MCI**

Thus, our future efforts will be focused on finding the structural variable(s) which can explain and quantify the soil sorption behavior of polar and ionic chemicals. Structural analysis of our results on polar and ionic compounds shows that their soil sorption capacity depends strongly on the presence and other factors have only minor influence on resulting soil sorption coefficient. The next developmental stage for the molecular connectivity model is to test its ability to predict the soil sorption coefficients of new, commercial chemicals that are registered at a very high rate. Their main structural characteristics are unusually large size and simultaneous presence of a large number and variety of functional groups. Such a trend will be emphasized even more in the future. Organic compound are used in many manufacturing process and in many products, exposure etc. Organic compound is mainly a manmade chemical, although it is found in nature in animal waste and organic material. The waste water contains various type of organic compounds as chloro, nitro, amino, and other substituted compounds. Various types of pesticides which are related to organic compound like organochlorines and organophosphates, various dyes also pollute the water. Adsorbent is a well stabilized technique for the treatment of industrial waste water. High cost and difficult procurement of activated Carbon in India has prompted search for suitable alternatives. Soil clay is very easily available adsorbent. The mode of operation in this study is batch type which is helpful to environment. But to predict toxicity and fat of chemicals QSAR has the capability to assist in the prioritization of chemicals for testing. QSAR are computer based mathematical models which give information about the properties of compounds (such as potential biological effect) on the basis of their chemical structure alone. It is also helpful for estimate the absorbability of untested chemicals in the absence of experimentation. Nowadays many QSAR models have been developed to predict soil/Carbon sorption, agrochemical, pharma, aquatic toxicity, drug chemicals etc. These studies may be helpful to environmental engineers for designing and establishing a continuous treatment plant for From the table no.1 it is clear that A review Representative examples of regression models used to estimate log organic carbon–normalized sorption coefficient (log KOC) from log octanol–water partition coefficient (log KOW)of the existing QSARs for predicting using the approach to estimate sorption coefficients will be presented.water enriched in organic compounds .Another area of interest in the field of environmental modelling is to develop molecular connectivity models that will predict sorption properties of commercial chemicals on other soil or sediment components (clay, sand, silt, swelling clay, etc.) and the wide variety of surfaces frequently encountered in the subsurface. When developed, these models will be extremely valuable, since the experimental data for such materials are exceptionally scarce. Over the past several decades, a variety of QSARs have been developed and evaluated for predicting sorption coeffi-cients for organic chemicals. Generally, each new generation of QSARs shows an incremental improvement over previous approaches because of the availability of new (and sometimes higher quality) experimental data, the increased statistical rigor associated with model validation, or through improved chemical descriptors generated via new computational techniques. However, despite the improvement in the number and type of chemical descriptors that have been used in QSAR development, almost all the new methods for estimating sorption coefficients have used the KOC approach, where sorption is expressed as a function of the organic carbon content of the sorbent.

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