PREDICTION OF GAS-PARTICLE PARTITIONING OF POLYCYCLIC AROMATIC HYDROCARBONS BASED ON M5' MODEL TREES

by

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During the thermal combustion processes of carbon-enriched organic compounds, emission of polycyclic aromatic hydrocarbons into ambient air occurs. Previous studies of atmospheric distribution of polycyclic aromatic hydrocarbons showed low correlation between the experimental values and Junge-Pankow theoretical adsorption model, suggesting that other approaches should be used to describe the partitioning phenomena. The paper evaluates the applicability of multivariate piece-wise-linear M5' model-tree models to the problem of gas-particle partitioning. Experimental values for particle-associated fraction, obtained for 129 ambient air samples collected at 24 background, urban, and industrial sites, were compared to the prediction results obtained using M5' and the Junge-Pankow model. The M5' approach proposed and models learned are able to achieve good correlation (correlation coefficient >0.9) for some low-molecular-weight compounds, when the target is to predict the concentration of gas phase based on the particle-associated phase. When converted to particle-bound fraction values, the results, for selected compounds, are superior to those obtained by Junge-Pankow model by several orders of magnitude, in terms of the prediction error.

Key words: *ambient air, high volume sampling, gas-particle partitioning,
polycyclic aromatic hydrocarbons, M5' model trees, data mining*

Introduction

During the thermal combustion processes of carbon-enriched organic compounds, different inorganic and organic compounds are generated, including dominantly polycyclic aromatic hydrocarbons (PAH). Since some individual PAH and their environmental mixtures show strong mutagenicity and carcinogenicity [1-4], they are of special concern in environmental research. PAH pose a danger to the environment and human health as they can be transported (mostly via air) over long distances [5, 6]. Among more than 100 different chemicals from the

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Radonić, R. J., *et al.*: Prediction of Gas-Particle Partitioning of Polyclyclic ...

552 THERMAL SCIENCE: Year 2012, Vol. 16, No. 2, pp. 551-560

group of PAH, some PAH are listed individually on United States Environmental Protection Agency's (EPA) Priority Chemical list [7].

Bombing and destruction during the war in former Yugoslavia (1991-1999), accompanied by complete and incomplete combustion, caused emission of large amounts of PAH into the atmosphere, water, and soil. Taking into consideration historical pollution and permanent generation of PAH at the urban sites (both industrial and residential), our investigation was based on experimental results from 24 background, urban, and industrial sites in Croatia, Bosnia and Herzegovina and Serbia, obtained within the FP5 EU Project *Assessment of the selected POPs in the atmosphere and water ecosystems from the waste materials generated by warfare in former Yugoslavia* (ICA2-CT2002-10007, see:
 http://www.recetox.muni.cz/projekty/apopsbal/).

Theory of gas-particle partitioning of SVOC/PAH

Gas-particle partitioning of semi volatile organic compounds (SVOC), including PAH, influences the fate, long-range transport, and transformation processes in the atmosphere and has been assessed in a number of recent theoretical and field studies [2, 3, 5, 8-13]. For the quantification of the gas-particle partitioning of SVOC, the partitioning coefficient K_p or particle-bound fraction ϕ are used. While ϕ is defined as ratio of compound concentration associated with the particle phase, F [ngm^{-3}], over the sum of gas A [ngm^{-3}], and particle concentrations, K_p is a ratio of *F/TSP* over A, where *TSP* [μgm^{-3}] is the total suspended particulate matter concentration .

For the prediction of the atmospheric distribution of SVOCs, the most frequently used model is an adsorption model proposed by Junge [14] and Pankow [15], which assumes that chemicals adsorb to the active sites on the surface of particles. It can be explained using the linear Langmuir isotherm:

$$\phi = \frac{F}{A + F} = \frac{c\theta}{p_L^0 + c\theta}$$

(1)

where θ [m^2 m^{-3}] is the particle surface area, p_L^0 [Pa] – the sub-cooled liquid vapour pressure and c [Pa·m] – the parameter which depends on the difference between the heat of desorption of the compound from the particle surface and the heat of vaporization, and the surface properties of the suspended particles.

Within the previous study aimed at understanding the partitioning behaviour of POP, including PAH, in the Balkan countries [3], experimental results were compared to those predicted using the Junge-Pankow model. Unfortunately, the obtained estimations differed significantly from the experimental values and the Junge-Pankow model was consider to be inadequate, especially for PAH of low molecular weight, suggesting that other approaches should be used to describe the process.

Data mining/knowledge discovery

Machine learning techniques [16] can be used to create models based on experimental data, rather than theoretical reasoning. The process is usually referred to as data mining or knowledge discovery. Although a large number of such approaches exist, many of them can deal only with the problem of classification and are unable to handle the task of predicting a numeric variable and are therefore unsuitable for the task of predicting the gas-particle partitioning of

Radonić, R. J., *et al.*: Prediction of Gas-Particle Partitioning of Polycyclic ...
THERMAL SCIENCE: Year 2012, Vol. 16, No. 2, pp. 551-560

553

PAH. The approaches that can be used for this purpose include standard regression, neural networks, instance-based learning, and regression trees [17]. Standard regression imposes linear relationship on the data and is therefore of limited applicability. The neural networks and instance-based learning are much more powerful but suffer from the problem of opacity; the models do not reveal anything about the structure of the function learnt and therefore provide no insight into the nature of the problem to the human experts. Regression trees combine the descriptive power of the decision tree approach with the numeric prediction, but the function they are able to model is a piece-wise constant one [18].

Model trees, such as those learned by the M5' approach [17], used in the study described below, are piece-wise linear models that combine conventional decision trees with linear regression functions at the leaves. The tree building algorithm splits the data into clusters of sufficiently low variance. It then proceeds to replace parts of the decision tree with linear regression functions. An example of an M5' tree, that attempts to model a sine function, is shown in fig. 1. To keep the model shown simple the only parameter supplied to the algorithm – minimum number of instances that will be covered by each leaf node – has been set a very high value, resulting in a fairly inaccurate approximation. Starting from the top, each oval node represents a decision based on the value of the attribute denoted in the node. The values used in the decision are shown on the corresponding branches. The squares in fig. 1 denote the leaf nodes that contain linear models (LM1-LM3). To calculate the value of the sine function for a specific input value *x*, based on the model shown in fig. 1(a), the appropriate linear model is selected by testing the value of *x* is against the conditions associated with each successive branch, starting form the root node. Once the linear model is selected, it is used to calculate the modelled value for sine. The leaf nodes shown in fig. 1(a) show the number of training instances (input values) covered by the associated linear model and the root relative squared error for that model. The three linear models form the piece-wise model which is plotted against real sine function values in fig. 1(b).
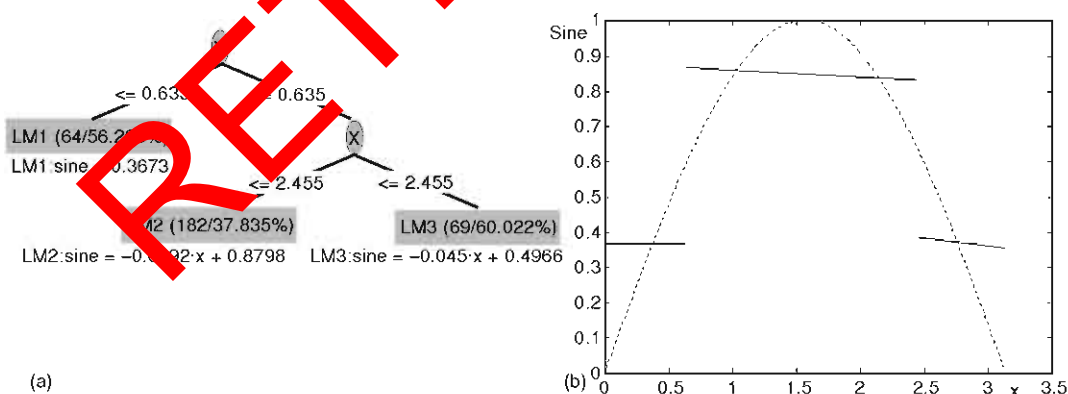

Figure 1. Simple M5' model of a sine function (a) and a plot of model predicted values against the accurate sine value (b)

In the context of modelling gas-particle distribution, when a new set of particle-bound concentration measurements is obtained, a learnt model can be used to predict the value of a compound in the gas phase.

554

Radonić, R. J., *et al.*: Prediction of Gas-Particle Partitioning of Polycyclic ...
THERMAL SCIENCE: Year 2012, Vol. 16, No. 2, pp. 551-560

Rather than relying on single-compound particle-bound values to predict the gas phase, the models consider particle-bound data available for all the compounds monitored. In addition, due to the fact that sensors that can be used to monitor particle-bound phase are inexpensive when compared to gas phase monitoring devices, the models can be used to extend the areas monitored with the same financial resources, by making some of the gas-phase-monitoring sensors redundant.

The main objective of this study was to assess the applicability of data-driven modelling, as usually done in data mining, to the problem of gas-particle partitioning of PAH in the ambient air samples collected during the high volume sampling campaign in the countries of former Yugoslavia.

The rest of the paper is organized as follows: section 2 deals with the materials and methodology applied, section 3 is dedicated to results obtained and the discussion, while section 4 holds our conclusion.

Materials and methodology

Data set collection

A total number of 129 air samples has been obtained from 24 sampling sites in three countries. Ten samples were collected from each of the sites in Croatia. Four samplers were positioned in the city of Zadar, Croatia – urban area (Z1 and Z4), industrial zone (Z2), and heavily contaminated area (Z3). Background sample was at the Zavižan location, mountain Velebit (ZAV). Five samples were taken from each of five sites in Sarajevo, Bosnia and Herzegovina – industrial zone (S1, S3, and S4), residential area (S2), and background site (S5) and another five sampling sites in Tuzla, Bosnia and Herzegovina – industrial area (T1 and T5), heavily contaminated zone (T2), residential area (T3) and background site (T4)). In Serbia, Kragujevac (industrial zone (K1 and K2), and urban area (K3), Pancevo – industrial area (P1 and P2) and urban locality (P3)) and Novi Sad (industrial zone (N1), residential part (N2) and urban area (N3) were the cities of interest, each providing three sampling sites and three air samples from each site. All samplers were placed on the ground, except at the point P3 where the roof of an eight-floor building has been used as the location of the sampling device. Samples were taken in the early summer period of 2003 and 2004, under comparable meteorological conditions at all sites, with median temperature 19 °C. High volume ambient air samplers PS-1 (Graseby-Andersen, USA, flow: 20-25 m^3/h, volume: 250-300 m^3 per 24 hours) and two types of sorbents were used: a Whatmann quartz filter for collection of particles, and a polyurethane foam (PUF) filter for collection of the gaseous phase. Duration of sampling was 24 hours. Before the campaign, PUF filters were extracted with acetone and dichloromethane in a Soxtec extractor, while quartz filters were heated to 450 °C [3].

Collected samples were extracted with dichloromethane in a Büchi System B-811 automatic extractor. One laboratory blank and one reference material were analyzed with each set of samples. Surrogate recovery standards (D8-naphthalene, D10-phenanthrene, D12-perylene) were spiked on each filter prior to extraction. Terphenyl was used as internal standards for PAH analyses. Volume was reduced after extraction under a gentle nitrogen stream at ambient temperature. The fractionation achieved on a silica gel column (30 cm length, 1 cm i. d.) was then used for the chemical analysis of the contents of 16 PAH. The samples were analyzed using GC-MS instrument (HP 6890-HP 5972) supplied with a J&W Scientific fused silica column DB-5MS [3]. All analytical procedures were done in the laboratories of Research Centre for

Toxic Compounds in the Environment, RECETOX, Masaryk University, Brno, Czech Republic.

Modelling methodology

The modelling methodology used in the study relies on the M5' approach described by Wang *et al.* [17]. The implementation of their approach is part of an open source data mining software package: Waikato Environment for Knowledge Analysis – WEKA [16]. For each compound the values of concentration in the gas phase were used as a target (dependent) variable, while the particulate phase values were used as the basis for prediction. A separate model was built for each compound. 10-fold cross-validation was used to evaluate the model performance, by randomly selecting 10% of the measurements to serve as the test set and building the model using the rest of the data. The process was repeated 10 times and average values of error rates are reported below. The only parameter provided to the M5' algorithm was the least number of instances covered by each node, which was set to 4.

Results and discussion

Junge-Pankow model

Using the Junge-Pankow model, the theoretical particle-bound fraction, ϕ, was calculated from eq. (1). Since a majority of sampling sites were urban or industrial facilities, calculations were performed assuming that $c = 0.172$ Pa·m and $\theta = 1.1 \cdot 10^{-3}$ m^2/m^3 [14], which are representative values for urban aerosols. Sub-cooled liquid vapour pressure at 298 K [19, 20] was applied for all compounds and roughly corresponded to the median temperature during the sampling campaigns.

Very good agreement between measured and modelled ϕ values was confirmed for higher molecular weight PAH (starting with chrysene). Modelled ϕ values were slightly underestimated (less than one order of magnitude) for phenanthrene, anthracene, fluoranthene and benzo[a]anthracene. Underestimation in the range from one to one and a half order of magnitude was observed for low molecular weight PAH (acenaphthylene, acenaphthene, and fluorene) with maximum of three orders of magnitude for naphthalene. A box plot of the prediction errors of the model for some low-molecular-weight PAH is shown in fig. 2. The plot shows median values and variability of values obtained for: acenaphthylene (Acy), acenaphthene (Ace),

Figure 2. Prediction performance of Junge-Pankow models for low molecular weight PAH

naphthylene (Acy), acenaphthene (Ace), fluorene (Flo), and phenanthrene (Phe). The sampling artefacts (break-through of the most volatile compounds decreasing the amount of captured gaseous chemicals, and sorption of the gaseous substances on the quartz filter increasing the sum of particle-bound chemicals) can be, at least partially, responsible for this discrepancy [3].
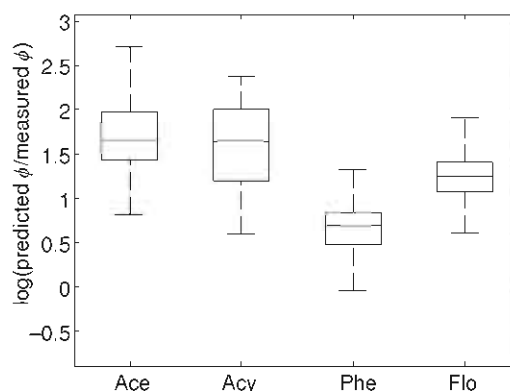
556

Radonić, R. J., *et al.*: Prediction of Gas-Particle Partitioning of Polycyclic ...
THERMAL SCIENCE: Year 2012, Vol. 16, No. 2, pp. 551-560

M5' models

M5' models were trained to estimate compound concentration in the gas phase, A [mng^{-3}]. An estimation of the theoretical particle-bound fraction, ϕ, can be calculated using the estimated concentration and the known concentration associated with the particle phase. A separate model was trained for each compound and the concentration values in the dataset were normalized to enable interpretation of the linear regression models. The models were considered valid if the cross-validated correlation of the predictions was high (higher than 0.8). Here we present models obtained for acenaphthylene, acenaphthene, fluorene and phenanthrene where the correlation was higher than 0.88.

The correlation between the estimated and true values, various error rates and the number of rules and variables for the four models are listed in tab. 1. The errors rates listed correspond to mean absolute error (MAE), relative absolute error (RAE) and root relative squared error (RRSE). As the table shows the models are able to predict the value of the concentration of gas phase with the RAE rate of less than 50%.

Table 1. Correlation between estimated and true values, error rates, number of rules and variables

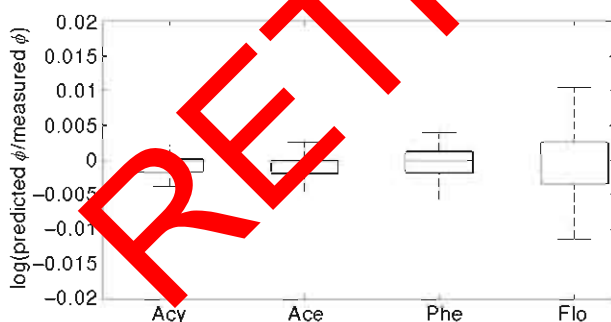| Compound	Correlation	MAE	RMSE	RAE [%]	RRSE [%]	Rules	Vars
Acy	0.9157	0.7601	1.6172	38907	40.0068	4	8
Ace	0.8868	0.1008	0.15 4	43.368	45.9515	1	13
Flo	0.9491	1.0385	1.6205	30.01	31.3434	1	11
Phe	0.9001	3.7 3	6174	36.7862	43.4603	1	9

Figure 3. Prediction performance of M5' decision tree models for low molecular weight PAHs

In order to evaluate a consistency between the particle-bound fractions predicted by the M5' models and the ones derived from the field measurements, the ratios between the field, and predicted ϕ values ($\log\phi_{measured}/\phi_{predicted}$) were plotted. Median value of this ratio and its variability can be seen in fig. 3 for these compounds.

Very good agreement was confirmed for low molecular weight PAH (acenaphthylene, acenaphthene, fluorene, and phenanthrene). The models are able to capture the dependencies that cannot be modelled accurately by the Junge-Pankow model [3]. These have been previously attributed, in part, to the sampling artefacts (break-through of the most volatile compounds decreasing the amount of captured gaseous chemicals, and sorption of the gaseous substances on the quartz filter increasing the sum of particle-bound chemicals).

Statistical significance of the differences between the predictions obtained by Junge-Pankow and the proposed models has been tested using two-tailed t-tests, which returned

significance levels of $9.77 \cdot 10^{-19}$, $7.72 \cdot 10^{-19}$, $4.36 \cdot 10^{-13}$, and $5.81 \cdot 10^{-40}$ for acenaphthylene, acenaphthene, fluorene, and phenanthrene. The values are well below the usual 0.05 significance level usually used to test for distribution difference, and prove that the error characteristics of the two models are indeed different. It should be noted that the both measured and M5' predicted values for the concentration of fluorene were occasionally zero. Since the error measure is undefined in such cases, the predicted values have been ignored in the plots and set to a very small concentration of the gas phase (10^{-5}) to enable statistical testing.

Gas-particle partitioning model for acenaphthylene

Only one decision tree, the model built for acenaphthylene and shown in fig. 4, was not reduced to a single regression equation. The decisions of which regression equation to use are, in this case, made based on the concentration of the particle-associated acenaphthylene (Acy) and benzo[a]anthracene (B[a]A), suggesting a strong link between the concentrations of these two compounds. Benzo[a]anthracene affects the choice of model for concentrations of particle-associated acenaphthylene over 0.0115 ng/m³ (over the normalized value of 0.125), but seems to have little bearing on the selection of model for the concentrations of particle-associated acenaphthylene below this value. Two different linear models (LM3 and LM4 in fig. 3) were induced for high acenaphthylene values: LM3 for B[a]A concentration below 2.197 ng/m³ (normalized value 0.366) and LM4 for higher concentration.

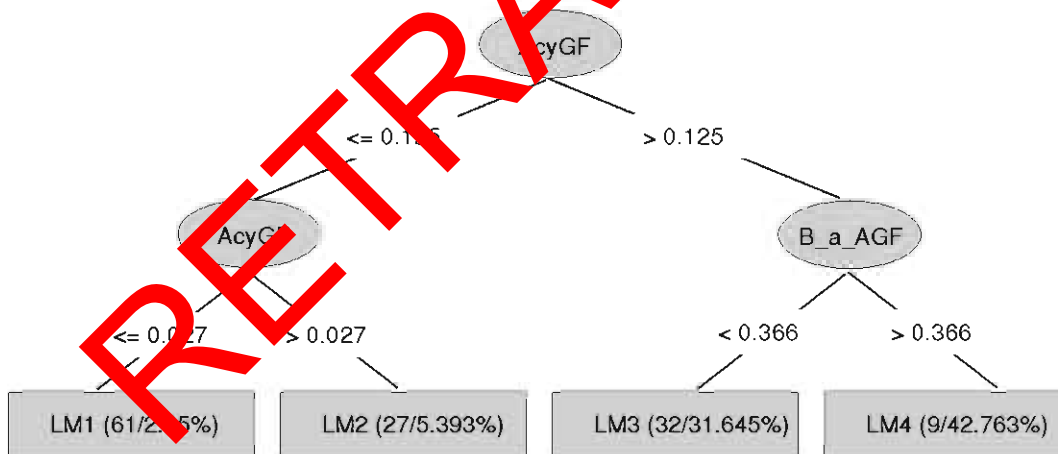
Figure 4. M5' model learned for acenapthylene

Table 2 provides the listing of the four linear models pertinent to acenaphthylene. As the table shows, the dominant factor in all the regression equations is the concentration of B[a]A. In addition, since our learning scheme treats the only nominal attribute (location) as binary, all models incorporate a factor specific to the group of locations in Bosnia and Herzegovina T1-T4 and S1. This is due to high concentrations of acenaphthylene in these sites and in accordance with the results of the cluster analysis performed in [3].

Table 2. Four linear models pertinent to acenaphthylene

LM1	AcyPUF = 0.0022·NapGF + 0.0643·AcyGF − 0.0112·FloGF − 0.0296·PheGF − 0.0321·AntGF + 0.0542·FluGF + **0.123·B_a_AGF** − 0.0438·I_123cd_PGF + 0.0007·location = Z4, K1, K3, Z3, Z5, K2, Z1, N3, Z2, S5, S3, S4, T5, S2, T4, S1, T3, T1, T2 + 0.0006·location = Z5, K2, Z1, N3, Z2, S5, S3, S4, T5, S2, T4, S1, T3, T1, T2 + 0.0043·location = T4, S1, T3, T1, T2 + 0.0049
LM2	AcyPUF = 0.0195·NapGF + 0.0908·AcyGF − 0.0112·FloGF − 0.0296·PheGF − 0.0321·AntGF + 0.0542·FluGF + **0.123·B_a_AGF**, − 0.0438·I_123cd_PGF + 0.0012·location = Z4, K1, K3, Z3, Z5, K2, Z1, N3, Z2, S5, S3, S4, T5, S2, ⬚, S1, T3, T⬚ T2 + 0.0107·location = Z5, K2, Z1, N3, Z2, S5, S3, S4, T5, S2, T4, S1, T3, T⬚, T2 + 0.0043·location = T4, S1, T3, T1, T2 − 0.0005
LM3	AcyPUF = 0.2357·AcyGF − 0.0206·FloGF − 0.2575·PheGF − 0.0971·⬚GF + 0.328·FluGF + **0.4831·B_a_AGF** − 0.2197·I_123cd_P⬚ + 0.0434·location = T4, S1, T3, T1, T2 + 0.0189
LM4	AcyPUF = 0.1512·AcyGF − 0.0206·FloGF − 0.33⬚·PheGF − 0.1337·AntGF + 0.7463·FluGF + + **0.7292·B_a_AGF** − 0.4338·⬚123cd_PG⬚ + 0.0305·location = T4, S1, T3, T1, T2 − 0.0379

Gas-particle partitioning models for other compounds

Table 3 lists the models obtained for 3 other compounds (Ace, Flo, Phe), with predictions, once again, highly correlated with the measured values of gas-phase concentration. All models were reduced to a single regression equation by the learning algorithm. The highest single contributing factors to the prediction of gas-phase concentrations of acenaphthene, fluorene and phenanthrene are the particle-phase concentrations of fluoranthene (Flu).

Table 3. Models obtained for Ace, Flo and Phe

Compound	Model
Ace	AcePUF = 0.1088·NapGF + 0.2039·AcyGF + 0.1141·AceGF − 0.398·PheGF − 0.2⬚·AntGF + **0.8666·FluGF** − 0.4521·PyrGF + 0.7139·B_a_AGF + 0.2247·ChrGF + 0.3977·B_k_FGF − 6881·B_a_PGF − 0.1553·B_ghi_PGF + 0.0379·location = Z3, Z2, S5, K2, Z1, K1, S3, S4, S2, T5, T4, T3, S1, T1, T2 − 0.0439·location = K2, Z1, K1, S3, S4, S2, T5, T4, T3, S1, T1, T2 + 0.0367·location = Z1, K1, S3, S4, S2, T5, T4, T3, S1, T1, T2 + 0.0799·location = S1, T1, T2 − 0.0162
Flo	FloPUF = 0.0503·NapGF − 0.1598·AcyGF + 0.0389·AceGF + 0.1039·FloGF − 0.3612·PheGF + **0.9173·FluGF** − 0.5851·PyrGF + 0.74·B_a_AGF + 0.1494·B_b_FGF − 0.1215·B_k_FGF + 0.0248·location = N3, Z3, K1, Z1, K2, Z2, P1, P2, S5, S3, S2, S4, S1, T4, T5, T3, T1, T2 + 0.0548·location = S4, S1, T4, T5, T3, T1, T2 − 0.0053
Phe	PhePUF = − 0.3992·AcyGF + 0.187·AceGF − 0.1635·PheGF − 0.1765·AntGF + **0.6914·FluGF** − 0.3523·B_a_AGF + 0.2348·ChrGF + 0.6513·B_a_PGF + 0.1224·location = S2,K1,S1,P1,S4,K2,T4,T5,T3,P2,T1,T2 + 0.0431

Radonić, R. J., *et al.*: Prediction of Gas-Particle Partitioning of Polycyclic ...
THERMAL SCIENCE: Year 2012, Vol. 16, No. 2, pp. 551-560

559

Conclusions

It has been shown that partitioning behaviour of a compound between gaseous and particulate phases cannot be accurately predicted from the compound properties and ambient temperature using classical theoretical models. Although the Junge-Pankow model predicts the median value of particle-bound fraction of most compounds with the reasonable precision, variability of the results can range over several orders of magnitude.

The M5' approach proposed and models learned are able to achieve good correlation (correlation coefficient >0.88) for the 4 different compounds considered in this study, when the target is to predict the concentration of gas phase based on the particle-associated phase. When translated to particle-bound fraction values, the results, for selected compounds, are superior to those obtained by Junge-Pankow model in terms of the prediction error, by several orders of magnitude.

More information on the gas/particle partitioning can be gained by employing machine learning and knowledge discovery (data mining) techniques. The M5' model trees are able to utilize the interdependence between different PAH to predict the concentration of the gas-phase based on particle-phase data. The models learned are simple and suitable for interpretation by experts.

The improved performance of the relatively simple M5' models learned over the classical theoretical partitioning models suggest that they benefit from the additional information and, that, therefore, the theoretical models should be extended to take into account the interdependence of various PAH concentrations.

Acknowledgment

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560

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