APPLICABILITY OF REGRESSION TECHNIQUE FOR PHYSICAL MODELING: A CASE STUDY ON ADSORPTION IN WASTEWATER TREATMENT

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ABSTRACT

The reliability of Physical Modeling in applications such as Adsorption and Heat transfer studies is not accurate since their mechanisms are complex and a proper understanding of the physics of the system is incomplete. In order to verify the applicability of Regression technique for Physical Modeling, a physical model is developed based on Multiple regression technique to predict the Pollutant Removal efficiency of fluoride in adsorption studies. Two sets of data points are collected viz., of twenty-one points consisting of homogeneous data with respect to adsorbent and of forty-eight points (heterogeneous data, including the above twenty-one points) and tested with the model. Results showed that, the physical model is giving encouraging results for homogeneous data (Standard Deviation (SD): 0.157) but is giving erratic results (SD: 0.361) for the heterogeneous data. The heterogeneous data consists of non-linear adsorption data, which the model could not predict accurately indicating that, the Regression technique holds a limitation in understanding the physics of the system. Novel techniques such as ANN can be used to predict the output from the data set with better accuracy than that using Regression technique. Back propagation Network of ANN is used as a test trial for the above database and the results are encouraging (SD: 0.29) with respect to heterogeneous data.

Key Words: Physical Modeling, Adsorption, Fluoride Removal, Pollutant Removal Efficiency, Multiple Regression, Artificial Neural Networks.

INTRODUCTION

Physical modeling for any Engineering application is usually based on proposing empirical relations with large amount of experimental data and the relevant non-dimensional parameters using Regression techniques. A number of sources are available in literature particularly in Environmental Engineering applications, where Regression technique is used for their data. For instance, Regression technique is used in Adsorption studies for the determination of kinetics of adsorption (Mohammad et al., 1997; [Patnaik and Das, (1995) and Khanna and Malhotra, (1977)]; for estimation of equilibrium time of adsorption [Bhargava and Killedar, (1991)]; prediction of removal efficiency of Cr (VI) under the specific range of the operating parameters tested [Manju and Anirudhan, (1997) and Raji and Anirudhan, (1997)]. A number of other applications of Regression technique are also found in the broad domain of Environmental Engineering for estimating the aspects such as: water quality parameters of River Thunga Bhadra [Aravinda et al., (1998)]; overall BOD removal rate in Ramganga river [Pande and Sharma, (1998)]; relation of different soil parameters with plant population, dry weight, and diversity index of communities on account of gas flaring at gas collecting stations [Rajkhowa et al., (1998)]; lethal concentration of copper to *Lepidocephalichthys Thermalis* fish [Geetha et al., (1996)]; hardness of water with respect to selected water quality parameters [Kumaresan and Kumari, (1996)]; water quality parameters for River Punnurpuzha [Abbasi et al., (1996)]; toxicity on bioaccumulation of cadmium and zinc in freshwater fish [Barber and Madhu, (1998)]; variation of fluoride content in underground water with respect to selected water

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quality parameters [Garg et al., (1998)] etc. The Regression technique is used to develop correlations between the mortality and lethality rates on crabs due to zinc and cadmium toxicity [Rao et al., (1998)] and the blood lead levels and ambient lead levels [Mooniaruck et al., (1996)]. Correlations based on regression technique are frequently used in Heat Transfer applications [Babu, (1993)].

However, the reliability of Physical Modeling in applications such as Heat transfer and Adsorption studies is not accurate since their mechanisms are complex and a proper understanding of the physics of the system is incomplete. For example, the efficiency of adsorption depends on several parameters and is predominantly material (adsorbent/adsorbate) specific. The parameters that are generated using experimental results are not adequate to develop an appropriate Physical Model since they fail in projecting a complete representation of adsorption mechanism. An alternate technique that can overcome the above limitations and function independent of the mechanism of a specific unit operation (eg. Adsorption) will be helpful for Engineering Applications.

CASE STUDY

The prediction of Pollutant Removal Efficiency (PRE) from effluent streams is an important criterion in Environmental Engineering Applications for decision making with regard to planning, design, and monitoring Pollution Control operations. In order to study the capability of Regression techniques for predicting the efficiency of adsorption, the prediction of PRE by adsorption in wastewater treatment is considered as a case study. In the present study, a Physical Model is developed based on affecting parameters in conjunction with Multiple Regression (PMMR) to predict the removal of Fluoride from contaminated water by adsorption.

RESULTS AND DISCUSSION

A compiled database available in literature consisting of twenty-one data points [Bhargava, (2002)] pertaining to the same adsorbent (homogeneous with reference to the adsorbent) is collected. The database has three independent variables viz., Initial concentration of the adsorbate, Adsorbent dose, & Contact time, and one dependent variable viz., PRE. The PMMR is developed in the present study using Matlab software [Rudrapratap, (1999)] and Microsoft Excel. The PMMR is developed using the database and validated by comparing the predicted data with that of the actual data. The accuracy of the prediction is determined using Standard Deviation (SD) calculated with reference to the actual data. The SD used in the present study is determined using the following formula [Babu, (1993)]:

$$S.D = \sqrt{\frac{\sum_{1}^{n}\left[\frac{y_{expected} - y_{calculated}}{y_{expected}}\right]^2}{n-1}}$$

The results indicated that the predicted data is in close agreement with that of actual data and gave a SD of 0.157.

The model is tested by adding another database of twenty-seven data points [Mariappan and Vasudevan, (2002)] generated for another adsorbent but for the same pollutant totaling to forty-eight data points. The second database of twenty-seven data points comprises of non-linear data points generated during the batch studies of adsorption. The data thus developed is heterogeneous, which is fitted in the PMMR to verify the validity of the model for heterogeneous and non-linear adsorption data. Interestingly, it is found that the prediction of the model for this combined data is relatively erratic and a SD of 0.361 is recorded. This corresponds to an increase of 130% than that for a homogeneous data. The details are given in Fig.1. The range of the input and output variables studied are given in Table-1.

Table-1. Range of variables studied

Variable	Upper limit	Lower limit
Initial Concentration of adsorbate, mg/L	30	3
Adsorbent dose, g/L	32	1
Contact time, min	960	5
PRE, %	95.1	20

From the Fig. 1, it can be noted that, many of the calculated values are in resemblance with those of actual values except for a small zone of database. This zone corresponds to the equilibrium values of adsorption, having approximately the same value. The physics of the adsorption system could not be adequately explained by the dimensional variables considered in PMMR and gave highly deviating values for this zone. Such types of equilibrium adsorption values are not available in the first data set and hence the deviation is comparatively lesser resulting in a lower SD value.

The study showed that the Physical Modeling based on affecting dimensional variables in conjunction with Regression Techniques does not always ensure good prediction unless and until all the affecting variables or affecting dimensionless groups are identified. The success of physical modeling is highly dependent on the thorough understanding and complete knowledge of the physical phenomenon that is taking place in the given system. The present study proved that Regression Techniques have the limitation in accurately predicting the output due to incomplete understanding of physical phenomena. Under these circumstances, one has to try the novel techniques such as Artificial Neural Networks (ANNs), which can serve as an alternative and can be successfully applied for Physical Modeling purposes. A three layer Backpropagation Network of ANN is developed in C++ [Babu et al., (2002)] and is used as a *test trial* to verify the accuracy of PMMR's prediction. The learning parameters adopted in the present study are given in Table-2.

Table-2. Learning parameters used in ANN

S. No.	Learning parameter	Range
1	Number of Neurons in Hidden Layer (NNHL)	3, 5
2	Learning Rate (LR)	0.5, 0.7
3	Epochs	10000, 20000 to 100000 @ 20000 epochs
4	Error Tolerance (ET)	0.01

A SD of 0.26 is observed for the following combination of learning parameters: NNHL: 3; LR: 0.7; Epochs: 20000; and ET: 0.01. The SD value observed is encouraging compared to that obtained using PMMR for heterogeneous data. Babu et al., (2002) reported that ANN is giving encouraging results for heterogeneous data in adsorption studies. Basheer and Najjar (1996) reported successful application of ANN to column studies of adsorption consisting of homogeneous data.

SUMMARY AND CONCLUSIONS

A physical model is developed based on Multiple regression technique to predict the PRE of fluoride in adsorption studies. Data available from literature is used for this purpose. Two sets of data points are collected viz., of twenty-one points consisting of homogeneous data with respect to adsorbent and of forty-eight points (heterogeneous data, including the above twenty-one points) and tested with the model. Results showed that, the physical model is giving encouraging results for homogeneous data but is giving erratic results for the heterogeneous data. The heterogeneous data consists of non-linear adsorption data, which the model could not predict accurately indicating the physics of the system could not be adequately explained by the dimensional variables considered in the study. Novel techniques such as ANN can be used to predict the output from the data set with better accuracy than that using Regression technique. Results of the test trial for the above database using ANN are encouraging. Literature review indicates that ANN gives encouraging results to a heterogeneous and non-linear adsorption data.

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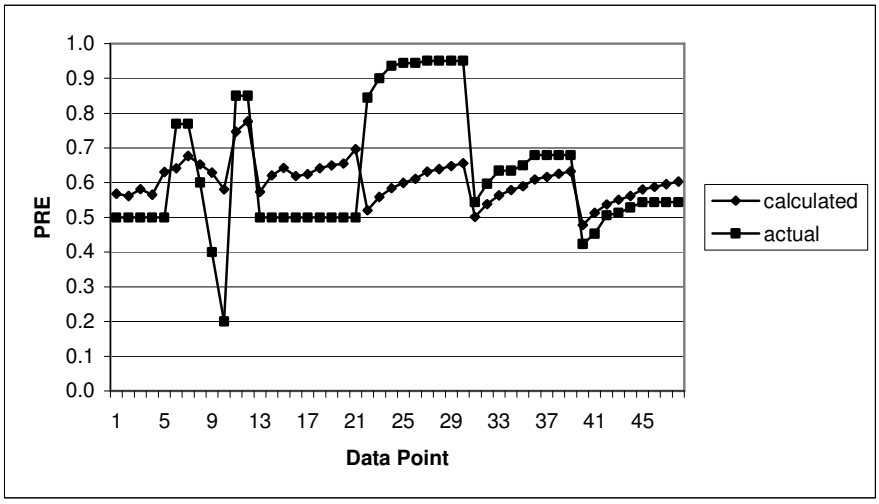

Fig. 1 Comparison of PRE for Multiple Variable Regressed Heterogeneous data