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Modeling Oxygen-transfer by Multiple Plunging Jets using Support Vector Machines and Gaussian Process Regression Techniques

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***Abstract*—**The paper investigates the potential of support vector machines and Gaussian process based regression approaches to model the oxygen–transfer capacity from experimental data of multiple plunging jets oxygenation systems. The results suggest the utility of both the modeling techniques in the prediction of the overall volumetric oxygen transfer coefficient (K_La) from operational parameters of multiple plunging jets oxygenation system. The correlation coefficient root mean square error and coefficient of determination values of 0.971, 0.002 and 0.945 respectively were achieved by support vector machine in comparison to values of 0.960, 0.002 and 0.920 respectively achieved by Gaussian process regression. Further, the performances of both these regression approaches in predicting the overall volumetric oxygen transfer coefficient was compared with the empirical relationship for multiple plunging jets. A comparison of results suggests that support vector machines approach works well in comparison to both empirical relationship and Gaussian process approaches, and could successfully be employed in modeling oxygen-transfer.

***Keywords*—**Oxygen-transfer, multiple plunging jets, support vector machines, Gaussian process.

I. Introduction

AN activated sludge process is the most widely preferred aerobic method of wastewater treatment. It is a biochemical process in which the rate of consumption of organic matter by the aerobic microorganisms is dependent upon the amount of available dissolved oxygen. In activated sludge process, oxygenation facility is designed to supply the required oxygen demand and to keep the return sludge-floc aerobic, as well as to provide adequate mixing so that there is an increase in contact opportunity between the microorganisms and the organic matter to enhance biological activity. Thus, one of the most important aspects of designing an activated sludge process system is concerned with the type and design of an oxygenation system.

Plunging jet applications include aeration and floatation in water and wastewater treatment, bubble floatation of minerals, oxygenation of mammalian-cell bio-reactors, biological aerated filter, fermentation, stirring of chemicals as well as increasing gas-liquid transfer, cooling system in power plants, plunging columns, breakers and waterfalls [1]-[7]. For aerobic treatment processes, such as activated sludge process, plunging jet oxygenation systems provide a simple and inexpensive method of supplying oxygen for wastewater treatment [1], [7], [8]. Oxygenation by a plunging water jet is an attractive way to effect oxygen-transfer than conventional oxygenation systems for various reasons[1], [7], [9], [10]: it does not require compressor blower; it facilitates make-up of the "closed" system, which enhance complete utilization of oxygen and volatile reactants; it is simple in design, construction and operation; it does not require separate stirring devices because the water jet itself achieves aeration and mixing; it is energetically attractive as a means of straightforward contacting mechanism in fouling or hazardous environments; and it is free from operational difficulties such as clogging in air diffusers, limitations on the installation of mechanical aerators by the tank width, etc. Supported by these potential advantages, there has been a growing interest in the oxygenation by plunging water jets in the last few years.

A number of studies have been reported on air-water oxygen transfer by single plunging jets [8], [11]-[18]. Some of these studies have also suggested empirical relationships between various jet parameters for estimating oxygen transfer capacity. The simplest relationships for single circular water jets plunging vertically as proposed by [19], [15] and [14] respectively are:

$$K_L A_{(20)} = 3.1\times10^{-4} + 4.85\times10^{-2} v_j^3 d_j^2 \quad (1)$$

$$K_L A_{(20)} = 9\times10^{-5} P \quad (2)$$

$$K_L A_{(20)} = 0.029\left(P/V\right)^{0.65} \quad (3)$$

where $K_L A_{(20)}$ is volumetric oxygen transfer factor at standard conditions (m^3/h); v_j is jet velocity at exit (m/s); d_j is jet diameter (m); P is jet power (W); $K_L A_{(20)}$ is volumetric oxygen transfer coefficient at standard conditions (1/s); and P/V is jet power per unit volume (kW/m^3).

Recently, [20] investigated oxygen-transfer by multiple plunging jets. The results showed that the volumetric oxygen-transfer coefficient at standard conditions ($K_L A_{(20)}$) and oxygen-transfer efficiency (OTE) for multiple-plunging-jets was higher than that for a single jet at a given jet power. Further, for multiple plunging jets device, the volumetric

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oxygen-transfer coefficient gradually increases as the number of jets was increased from 1 to 16. The study has recommended the use of multiple plunging jets device over single plunging jet system for aeration/oxygenation at higher jet powers as in practical situations where large volumes of wastewater at higher discharges are to be oxygenated. Deswal and Verma [20] have also suggested an empirical relationship for multiple plunging jets oxygenation systems as under:

$$K_L a_{(20)} = 0.113\ n^{0.84}\ v_j^{2.14}\ d_j^{1.53} \quad (4)$$

where, $K_L A_{(20)}$ is the volumetric oxygen-transfer coefficient at standard conditions (per sec) and n is the number of jets in multiple plunging jets oxygenation system.

Within last few years, soft computing techniques like artificial neural network, support vector machines, Gaussian processes and M5 model tree have been used in civil and environmental engineering applications [6], [21]-[31] and found to be working well.

Keeping in view the potential of Gaussian processes and support vector machines based regression approaches; the present study explores the capabilities of these techniques in modeling oxygen-transfer by multiple plunging jets and compares their performance with the empirical relationship suggested by [20].

II. Gaussian Process Regression

The Gaussian processes (GP) regression models are based on the assumption that adjacent observations should convey information about each other. Gaussian processes are a way of specifying a prior directly over function space. This is a natural generalization of the Gaussian distribution whose mean and covariance is a vector and matrix, respectively. The Gaussian distribution is based over vectors, whereas the GP is based over functions. Thus, due to prior knowledge about the data and functional dependencies, no validation process is required for generalization and GP regression models are able to understand the predictive distribution corresponding to test input [32].

A GP is defined as a collection of random variables, any finite number which has a joint multivariate Gaussian distribution. Let $\chi \times \gamma$ represent the domain of inputs and outputs respectively, from which n pairs (x_i, y_i) are drawn independently and identically distributed. For regression assume that $y \subseteq \Re$, then a GP on χ is defined by a mean function $\mu: \chi \to \Re$ and covariance function $k: \chi \times \chi \to \Re$.

The main assumption of GP regression is that y is given by $y = f(x) + \xi$ where $\xi \sim \mathrm{N}(0, \sigma^2)$. The symbol ~ in statistics means *sampling for*. In GP regression, for every input x there is an associated random variable $f(x)$, which is the value of the stochastic function f at that location. In this work it is assumed that observational error ξ is normal independent and identically distributed with mean value as zero ($\mu(x)=0$), variance σ^2 and $f(x)$ is drawn from the Gaussian process on χ specified by k. That is,

$$Y = (y_1, ..., y_n) \sim \mathrm{N}(0, K + \sigma^2 \mathbf{I})$$

where $K_{ij} = k(x_i, x_j)$ and $\mathbf{I}$ is the identity matrix.

Since $Y/X \sim \mathrm{N}(0, K + \sigma^2 \mathbf{I})$ is normal, so is the conditional distribution of test labels given training and test data $p(Y_*/Y, X, X_*)$. Then, one has $Y_*/Y, X, X_* \sim \mathrm{N}(\mu, \Sigma)$ where

$$\mu = K(X_*, X)\left(K(X, X) + \sigma^2 \mathbf{I}\right)^{-1} Y \quad (5)$$

$$\Sigma = K(X_*, X_*) - \sigma^2 \mathbf{I} - K(X_*, X)\left(K(X, X) + \sigma^2 \mathbf{I}\right)^{-1} K(X, X_*) \quad (6)$$

If there are n training data and n_* test data, then $K(X, X_*)$ represents the $n \times n_*$ matrix of covariances evaluated at all pairs of training and test data sets and similarly for the other values $K(X, X)$, $K(X_*, X), K(X_*, X_*)$; where X and Y is the vector of training data and training data labels y_i, whereas X_* is the vector of test data.

A specified covariance function is required to generate a positive semi-definite covariance matrix K, when $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$. The term kernel function used in SVM is equivalent to the covariance function used in GP regression. With the known values of kernel k and degree of noise σ^2, (5) and (6) would be enough for inference.

During the training process of GP regression models, one needs to choose a suitable covariance function as well as its parameters. In case of GP regression with a fixed value of Gaussian noise, GP model can be trained by applying Bayesian inference, that is maximizing marginal likelihood. This leads to the minimization of the negative log-posterior:

$$p(\sigma^2, k) = \frac{1}{2} \mathrm{y}^T \left(K + \sigma^2 \mathbf{I}\right)^{-1} \mathrm{y} + \frac{1}{2} \log \left|\mathrm{K} + \sigma^2 \mathbf{I}\right| - \log p(\sigma^2) - \log p(k) \quad (7)$$

To find the hyper-parameters, the partial derivative of (7) can be obtained with respect to σ^2 and k and minimization can be achieved by gradient descent. For further details about GP regression and different covariance function readers are referred to [33].

III. Support Vector Machines

Support vector machines (SVMs) are classification or regression methods, which have been derived from statistical learning theory [34]. The SVMs classification methods are based on the principle of *optimal separation* of classes. If the classes are separable – this method selects, from among the infinite number of linear classifiers, the one that minimize the generalization error, or at least an upper bound on this error, derived from structural risk minimization. Thus, the selected hyper plane will be one that leaves the maximum margin between the two classes, where margin is defined as the sum of the distances of the hyper plane from the closest point of

the two classes [34].

If the two classes are non-separable, the SVMs try to find the hyper plane that maximizes the margin and at the same time, minimizes a quantity proportional to the number of misclassification errors. The trade off between margin and misclassification error is controlled by a positive constant that has to be chosen beforehand. This technique of designing SVMs can be extended to allow for non-linear decision surfaces. This can be achieved by projecting the original set of variables into a higher dimensional feature space and formulating a linear classification problem in the feature space [34]. The support vector machines can be applied to regression problems and can be formulated as given below:

Reference [34] proposed Support Vector Regression (SVR) by introducing an alternative insensitive loss function (ε). This loss function allows the concept of margin to be used for regression problems. Purpose of the SVR is to find a function having at the most ε deviation from the actual target vectors for all given training data and have to be as flat as possible [35]. This can be put in other words as the error on any training data has to be less than ε. For a given training data with k number of samples, represented by $(\mathbf{x}_1, y_1),.....,(\mathbf{x}_k, y_k)$ a linear decision function can be represented by

$$f(\mathbf{x},\alpha) = \langle \mathbf{w}, \mathbf{x} \rangle + b \tag{8}$$

where $f(\mathbf{x},\alpha) \Rightarrow \alpha \in \Lambda$ (where Λ is a set of parameters used in the decision rule; for example, in a multilayer neural network, Λ is a set of weights of the network), $\boldsymbol{x}$ is an N dimensional observed data vector, R is set of all real numbers, b is the bias term that determine the offset of the hyperplane from origin and $\boldsymbol{w}$ determines the orientation of hyperplane. Further, $\langle \mathbf{w}, \mathbf{x} \rangle$ represents the dot product in space $\mathbf{R}^N$. A smaller value of $\boldsymbol{w}$ indicates the flatness of (8), which can be achieved by minimising the Euclidean norm as defined by $\|\mathbf{w}\|^2$ [35]. Thus, an optimisation problem for regression can be written as:

$$\text{minimise } \frac{1}{2}\|\mathbf{w}\|^2 \text{ subject to } \begin{cases} y_i - \langle \mathbf{w}, \mathbf{x}_i \rangle - b \le \varepsilon \\ \langle \mathbf{w}, \mathbf{x}_i \rangle + b - y_i \le \varepsilon \end{cases} \tag{9}$$

The optimisation problem in (9) is based on the assumption that there exists a function that provides an error on all training pairs which is less than or equal to ε. In real life problems, there may be a situation like one defined for classification by [34]. So, to allow some more error, slack variables $\xi, \xi^{'}$ can be introduced in (9), and the optimisation problem defined above can be rewritten as:

$$\begin{aligned} &\text{minimise } \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{k}\left(\xi_i + \xi_i^{'}\right) \\ &\text{subject to } y_i - \langle \mathbf{w}, \mathbf{x}_i \rangle - b \le \varepsilon + \xi_i \\ &\qquad \langle \mathbf{w}, \mathbf{x}_i \rangle + b - y_i \le \varepsilon + \xi_i^{'} \end{aligned} \tag{10}$$

and $\xi_i, \xi_i^{'} \ge 0$ for all i = 1, 2,……, k.

The parameter C is determined by the user and it determines the trade-off between the flatness of the function and the amount by which the deviations to the error more than ε can be tolerated. The optimisation problem in (10) can be solved by replacing the inequalities with a simpler form by transforming the problem to a dual space representation using Lagrangian multipliers [36].

The Lagrangian is formed by introducing positive Lagrange multipliers $\boldsymbol{\lambda}_i, \lambda_i^{'}, \eta_i, \eta_i^{'}$ where i = 1,….,k and multiplying the constraint equations by these multipliers, and finally subtracting the results from the objective function (i.e. $\|\mathbf{w}\|^2$). The Lagrangian for (10) can be written as:

$$\begin{aligned} L = \frac{1}{2}\|\mathrm{w}\|^2 + C\sum_{i=1}^{k}\left(\xi_i + \xi_i^{'}\right) - \sum_{i=1}^{k}\lambda_i\left(\varepsilon + \xi_i - y_i + \langle \mathrm{w}, \mathrm{x}_i \rangle + b\right) \\ - \sum_{i=1}^{k}\lambda_i^{'}\left(\varepsilon + \xi_i^{'} + y_i - \langle \mathrm{w}, \mathrm{x}_i \rangle - b\right) - \sum_{i=1}^{k}\left(\eta_i \xi_i + \eta_i^{'} \xi_i^{'}\right) \end{aligned} \tag{11}$$

The solution of this optimisation problem can be obtained by locating the saddle point of the Lagrange function defined in the (11). The Saddle points of (11) can be obtained by equating partial derivative of L with respect to $\boldsymbol{w}$, b, ξ_i *and* $\xi_i^{'}$ to zero. Thus, (8) can now be written as:

$$f(\mathbf{x},\alpha) = \sum_{i=1}^{k}\left(\lambda_i^{'} - \lambda_i\right)\langle \mathbf{x}_i, \mathbf{x} \rangle + b \tag{12}$$

The technique discussed above can be extended to allow for non-linear support vector regression by introducing the concept of the kernel function [34]. This is achieved by mapping the data into a higher dimensional feature space, thus performing linear regression in feature space. The regression problem in feature space can be written by replacing $\mathbf{x_i} \cdot \mathbf{x_j}$ in (12) with $\mathbf{\Phi}(\mathbf{x_i}) \cdot \mathbf{\Phi}(\mathbf{x_j})$, where $\mathbf{\Phi}(\mathbf{x})$ is the mapping to the feature space.

Where $$\mathrm{K}(\mathbf{x_i}, \mathbf{x_j}) \equiv \mathbf{\Phi}(\mathbf{x_i}) \cdot \mathbf{\Phi}(\mathbf{x_j})$$

Regression function given in (12) can now be written as:

$$f(\mathbf{x},\alpha) = \sum_{i=1}^{k}\left(\lambda_i^{'} - \lambda_i\right) K(\mathbf{x}_i, \mathbf{x}) + b \tag{13}$$

IV. Data Set

Data used in the present study are taken from an earlier study by Deswal and Verma [20]. The study was reported that multiple plunging jets have higher oxygen transfer rate in comparison to a single jet under similar conditions. The study, as stated earlier, has also proposed an empirical relationship to predict the overall oxygen transfer coefficient ($K_L a$) by multiple plunging jets for a given configuration under required flow conditions (4). The dataset consists of forty four experimental observations on different configurations (in terms of jet diameter and number of jets) of multiple plunging jets oxygenation system. To predict the overall oxygen transfer coefficient by multiple plunging jets, three input parameters, namely jet velocity at exit (m/s), jet diameter (m) and number of jets was used. A ten-fold cross-validation was used with data points. Cross-validation is a method of estimating the accuracy of a regression model in which the input data set is divided into several parts (number defined by the user), with each part in turn used to test a model fitted to the remaining parts.

Design of SVMs and GP require selection of a suitable kernel. A radial basis function (RBF) kernel in SVMs has been found working well in several civil engineering applications [26]-[27], and thus used in this study. In order to have a uniform comparison, RFF kernel has been used in GP regression as well . The optimal values of various user-defined parameters for both support vector machines and GP are provided in Table I.

TABLE I
User-defined parameters

Approach	
Support vector machines	RBF kernel; C = 20; gamma = 2
Gaussian Processes	RBF kernel; Gamma = 0.5; noise = 0.04

V. Results

To assess the usefulness of SVMs and GP regression techniques in predicting overall oxygen transfer coefficient by multiple plunging jets, the dataset of [20] was used. The values of overall oxygen transfer coefficient obtained using (4) were also calculated for the dataset so as to compare it with SVMs and GP regression models. Correlation coefficient, coefficient of determination (R^2) and root mean square error (RMSE) values were used to compare the

TABLE II
Correlation coefficient and RMSE values

Approach	Correlation coefficient	Root mean square error
Support vector machines	0.971	0.002
Gaussian process regression	0.960	0.002
Empirical relationship (4) as proposed by [20]	0.961	0.003

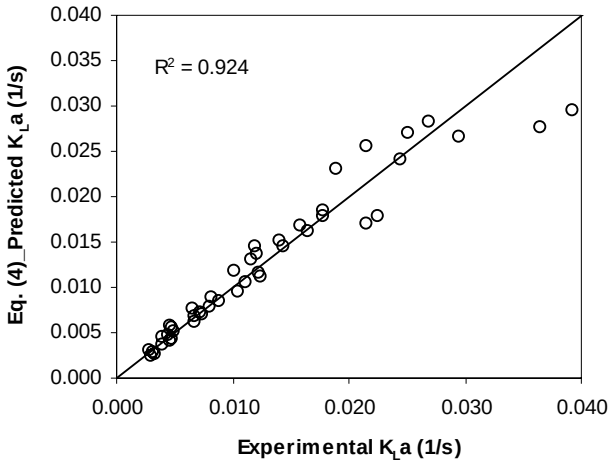

Fig. 1 Overall oxygen transfer coefficient by Eq. (4) proposed by [20] versus experimental data.

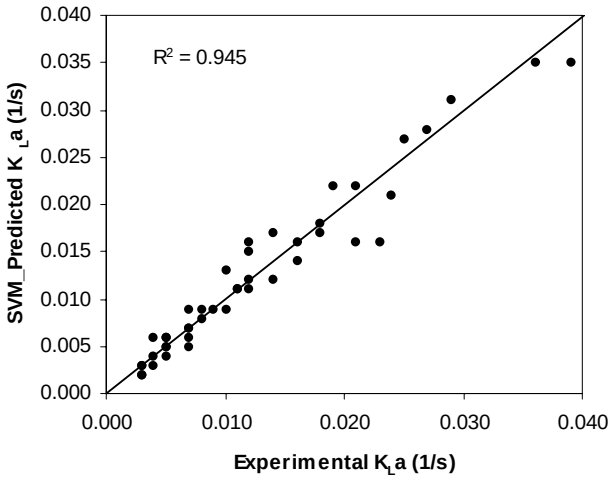

Fig. 2 Overall oxygen transfer coefficient by support vector machines versus experimental data.

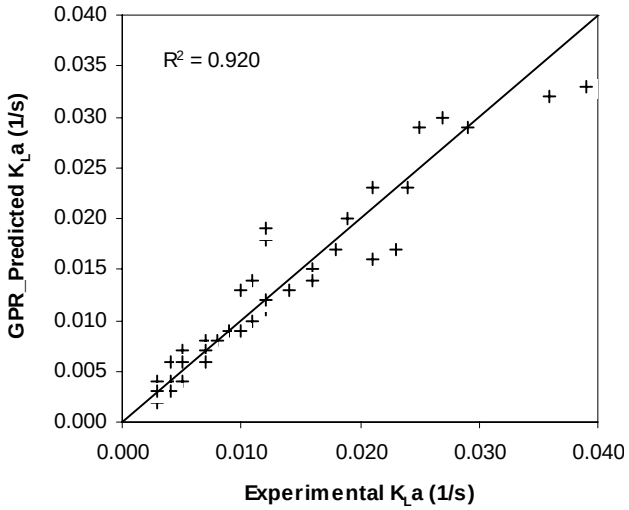

Fig. 3 Overall oxygen transfer coefficient by Gaussian process regression versus experimental data.

performance of SVMs and GP with empirical relationship proposed by Deswal and Verma [20] as represented by (4).

Table II provides values of correlation coefficient and RMSE obtained using SVMs, GP and empirical relationship (4) of [20]. In comparison to the correlation coefficient value of 0.961 (RMSE=0.003) achieved by empirical relationship (4), the GP and SVMs provide correlation coefficient values of 0.960 (RMSE=0.002) and 0.971 (RMSE= 0.002) respectively. Thus, suggesting the utility of both these regression techniques for such environmental engineering applications. However, the performance by SVMs is better than GP for this data set.

Figs. 1–3 provide the graphs plotted between experimental and predicted values of overall oxygen transfer coefficient by multiple plunging jets oxygenation system using empirical relationship (4) proposed by Deswal and Verma [20], SVMs and GP regression respectively. The SVMs results in Fig. 2 show less scatter in the data points than GP. Further, a higher value of R^2 (0.945) with SVMs confirms that this approach works well in predicting the overall oxygen transfer coefficient by multiple plunging jets in comparison to both the GP and empirical relationship (4) proposed by Deswal and Verma [20].

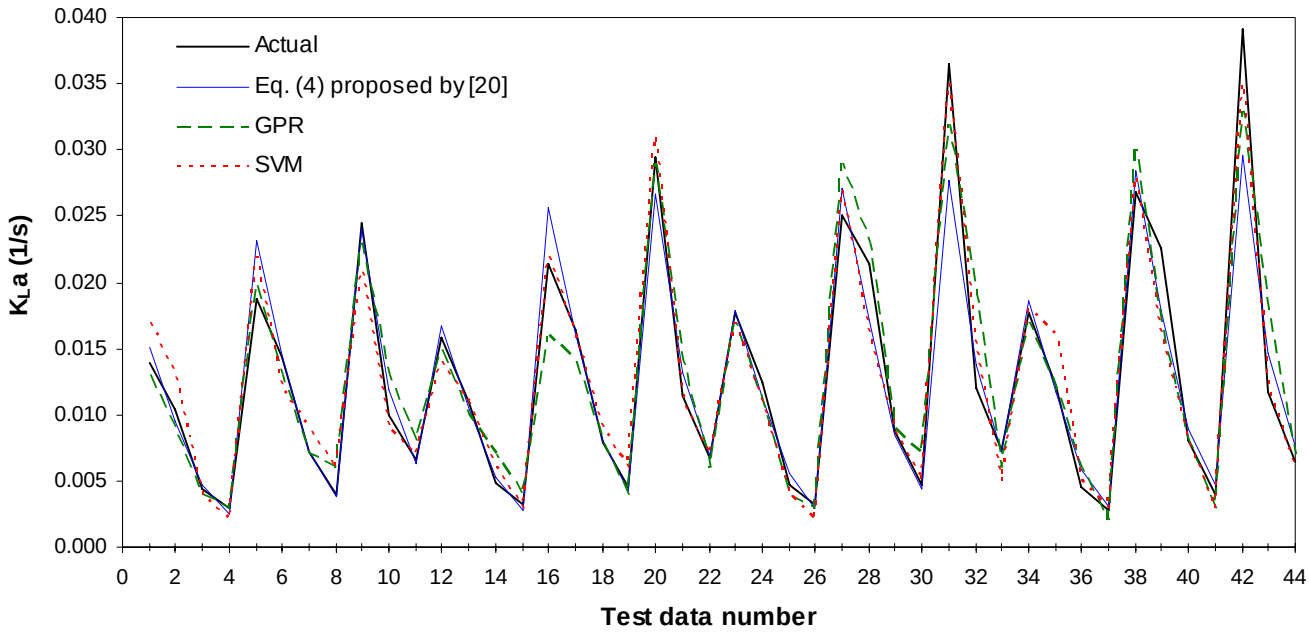

Fig. 4 Variation in predicted values by Eq. (4), GP and SVMs in comparison to the actual values of overall oxygen transfer coefficient by multiple plunging jets oxygenation system.

Fig. 4 represents the variation of experimental and predicted overall oxygen transfer coefficient by multiple plunging jets with the number of test data. It is evident from this plot that overall oxygen transfer coefficient predicted by SVMs regression technique is in good agreement with actual experimental values; whereas, that is not the case with GP regression approach as the predicted values by this technique are deviating at few of the test data. Thus, suggesting a better performance of SVMs in comparison to GP regression.

VI. Conclusion

This study has investigated the potential of SVMs and GP regression approaches in predicting overall oxygen transfer coefficient by multiple plunging jets oxygenation system in comparison with the empirical relationship suggested by [20]. The results presented are quite encouraging and suggest that the SVMs regression technique works well in comparison to GP regression for this data set but both of these approaches yields an approximation to the capacity predicted by empirical relationship. Further, the application of SVMs to such data can be utilized in comparing the performance of single and multiple plunging jets of different configurations and also in deciding the optimum configuration of multiple plunging jets for given flow conditions.

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