Computational techniques and their potential in predicting oxygen transfer by multiple oblique jets
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ABSTRACT
In last few years, there has been growing interest in the application of computational techniques to various areas of civil and environmental engineering. The paper investigates the potential of Gaussian Process, Neural Network and Support Vector Machines based regression approaches to model the oxygen-transfer capacity of multiple oblique jets oxygenation systems. These approaches are used in the prediction of the overall volumetric oxygen transfer coefficient from operational parameters of an oxygenation system having multiple oblique jets, number varying from 1 to 16, plunging at an impact angle of 60°. The results computed from these techniques and obtained from empirical relationship derived on the basis of multivariate linear regression are compared in terms of correlation coefficient, root mean square error and coefficient of determination. The results suggest the utility of these computational techniques in the designing and performance evaluation of plunging jets oxygenation systems; however, support vector machines have predicted overall volumetric oxygen transfer coefficient with highest correlation coefficient (0.985) and coefficient of determination (0.968), and lowest root mean square error (0.002) in comparison to other computational techniques as well as empirical relationship. Further, scattering (within ±10 percent) is lowest in case of support vector machines approach. A comparison of results suggests that support vector machines and neural network approaches work well and can be successfully used in modeling oxygen transfer from multiple oblique jets oxygenation systems.

Keywords: Oxygen transfer, multiple oblique plunging jets, support vector machines, Gaussian process, neural network.

1. Introduction
An activated sludge process is the most 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 oxygenation systems provide simple and inexpensive method that can be used in activated sludge process (Tojo et al., 1982; Bin, 1993; Deswal and Verma, 2007). Oxygenation by a plunging water jet is an attractive way to effect oxygen transfer than conventional oxygenation systems for several reasons (Kusabiraki et al., 1990; Bin, 1993; Emiroglu and Baylar, 2003; Deswal and Verma, 2007): it helps in making a “closed” system.
that enhance complete utilization of oxygen and volatile reactants; it is simple in design, construction and operation; it does not require compressor blower; it does not require separate stirring devices because the water jet itself achieves oxygenation 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 in the installation of mechanical aerators due to aeration tank dimensions; etc. Supported by these potential advantages, there has been a growing interest in the oxygenation by plunging water jets in the last few years.

Many studies have been reported on air-water oxygen transfer by a single jet plunging vertically, that is having an impact angle of $90^\circ$ (Ahmed, 1974; Van de Sande, 1975; Van de Donk, 1981; Bin and Smith, 1982; Tojo and Miyanami, 1982; Tojo et al., 1982; Bonsignore et al., 1985; Ohkawa et al., 1986; Funatsu et al., 1988). Some of these studies have also suggested empirical relationships between various jet parameters for estimating oxygen transfer capacity of a single jet. The simplest relationships for a single water jet plunging vertically are proposed by Ahmed and Glover (1972), Bin and Smith (1982) and Tojo and Miyanami (1982) and are given as under in the same order.

\[
K_L A_{(20)} = 3.1 \times 10^{-4} + 4.85 \times 10^{-2} v_j d_j^2 \\
K_L A_{(20)} = 9 \times 10^{-5} P \\
K_L a_{(20)} = 0.029 (P/V)^{0.65}
\]

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

Recently, Deswal (2008) investigated oxygen transfer by multiple oblique jets plunging at an impact angle of $\theta = 60^\circ$. The results showed that $K_L a_{(20)}$ and oxygen transfer efficiency for multiple oblique jets oxygenation system were about 1.5 times higher than that for a single oblique jet oxygenation system at a given kinetic jet power or similar flow conditions. Further, for multiple oblique jets oxygenation system, the volumetric oxygen-transfer coefficient gradually increases as the number of jets was increased from 1 to 16. The study has recommended the use of multiple oblique jets oxygenation system over a single oblique jet system for aeration/oxygenation at higher kinetic jet powers as in practical situations where large volumes of wastewater at higher discharges are to be oxygenated. Deswal (2008) has also suggested an empirical relationship, derived by using multivariate linear regression, between $K_L a_{(20)}$ and jet parameters for multiple oblique jets oxygenation systems as under:

\[
K_L a_{(20)} = 0.103 n^{0.81} v_j^{2.11} d_j^{1.43}
\]

where, $n$ is number of jets in a multiple oblique 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 (Chan et al., 1995; Chow et al., 1995; Dibike et al., 2001; Pal and
Mather, 2003; Deswal et al., 2006; Gill et al., 2006; Pal, 2006; Pal and Goel, 2006; Deswal and Verma, 2008; Pal and Deswal, 2008; Pal and Deswal, 2010) and found to be working well. Keeping in view the potential of Gaussian process, neural network and support vector machines based computational techniques; the present study explores the potential of these techniques in modeling oxygen-transfer by multiple oblique jets and compares their performance with the empirical relationship suggested by Deswal (2008).

2. Computational Techniques

2.1 Neural Network

A neural network (NN) is a form of artificial intelligence that imitates some function of the human brain. Neural networks are general-purpose computing tools that have the capability to solve complex non-linear problems. The network comprises of a large number of simple processing elements that are linked to each other by weighted connections according to a specified architecture. These networks learn from the training data by adjusting the connection weights (Bishop, 1995). There is a range of artificial neural network architectures designed and used in various fields. In this study, a feed-forward neural network with back propagation learning algorithm is used. The basic element of a back-propagation neural network is the processing node. Each processing node behaves like a biological neuron and performs two functions. First, it sums the values of its inputs. Second, the sum is then passed through an activation function to generate an output. Any differentiable function can be used as activation function, \( f \). All the processing nodes are arranged into layers, each fully interconnected to the following layer. There is no interconnection between the nodes of the same layer. In a back propagation neural network, generally, there is an input layer that acts as a distribution structure for the data being presented to the network. This layer is not used for any type of processing. After this layer, one or more processing layers follow, called the hidden layers. The final processing layer is called the output layer.

All the interconnections between each node have an associated weight. The values of the interconnecting weights are not set by the analyst but are determined by the network during the training process, starting with randomly assigned initial weights. There are many algorithms that can be used to adjust the interconnecting weights to achieve minimal overall training error in multi-layer networks (Bishop, 1995). The generalized delta rule or back-propagation (Rumelhart et al., 1996) is the most commonly used method. Back-propagation algorithm uses an iterative process to minimize an error function over the network output and a set of target outputs, taken from the training data set. The training data consists of a pair of data vectors. The training data vector is the pattern to be learned, and the desired output vector is the set of output values that should be produced by the network. The goal of training is to minimize the overall error difference between the desired and the actual outputs of the network. The training process begins with the entry of the training data to the network. The data flow forward through the network to the output units. At this stage, the network error (difference between the desired and actual network output) is computed. The network error is then fed backwards through the network towards the input layer with the weights connecting the units being changed in relation to the magnitude of the error. This process is repeated until the error rate is minimized or reaches an acceptable level, or until a specified number of iterations has been accomplished.
2.2 Support Vector Machines

Support Vector Machines (SVMs) are classification or regression methods. They trace their origin from statistical learning theory (Vapnik, 1995). 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 (Vapnik, 1995). If the two classes are non-separable: this method 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. It 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 (Vapnik, 1995). The support vector machines can be applied to regression problems and can be formulated as explained subsequently.

Support Vector Regression (SVR) was initially proposed by Vapnik (1995) with the introduction of an alternative insensitive loss function ($\varepsilon$). This loss function allows the concept of margin to be used for regression problems. The purpose of the SVR is to find a function having at the most $\varepsilon$ deviation from the actual target vectors for all given training data and have to be as flat as possible (Smola and Scholkopf, 1998). In other words, the error on any training data has to be less than $\varepsilon$. For a given training data with $k$ number of samples represented by $(x_1, y_1), \ldots, (x_k, y_k)$, a linear decision function can be represented by

$$f(x, \alpha) = \langle w, x \rangle + b \tag{5}$$

where $f(x, \alpha) \Rightarrow \alpha \in \Lambda$ (where $\Lambda$ is a set of parameters used in the decision rule; for example, in a multilayer neural network, $\Lambda$ is a set of weights of the network), $x$ 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 $w$ determines the orientation of hyperplane. Further, $\langle w, x \rangle$ represents the dot product in space $R^N$. A smaller value of $w$ indicates the flatness of equation (5), which can be achieved by minimizing the Euclidean norm as defined by $\|w\|^2$. Thus, an optimization problem for regression can be written as:

$$\text{minimize} \frac{1}{2} \|w\|^2 \quad \text{subject to} \quad \begin{cases} y_i - \langle w, x_i \rangle - b \leq \varepsilon \\ \langle w, x_i \rangle + b - y_i \leq \varepsilon \end{cases} \tag{6}$$

The optimization problem in equation (6) 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 $\varepsilon$. In real life problems, there may be a situation like one defined for classification by Vapnik (1995). So, to allow some more error, slack variables $\xi, \xi'$ can be introduced in equation (6), and the optimization problem defined above can be rewritten as:
minimize \( \frac{1}{2} \|w\|^2 + C \sum_{i=1}^{k} (\xi_i + \xi_i') \)

subject to \( y_i - \langle w, x_i \rangle - b \leq \varepsilon + \xi_i \langle w, x_i \rangle + b - y_i \leq \varepsilon + \xi_i' \)

and \( \xi_i , \xi_i' \geq 0 \) for all \( i = 1, 2, \ldots, k. \) (7)

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 \( \varepsilon \) can be tolerated. The optimization problem in equation (7) can be solved by replacing the inequalities with a simpler form by transforming the problem to a dual space representation using Lagrangian multipliers (Leunberger, 1984).

The Lagrangian is formed by introducing positive Lagrange multipliers \( \lambda_i , \eta_i , \eta_i' \), where \( i = 1, \ldots, k \) and multiplying the constraint equations by these multipliers, and finally subtracting the results from the objective function (i.e. \( \|w\|^2 \)). The Lagrangian for equation (7) can be written as:

\[
L = \frac{1}{2} \|w\|^2 + C \sum_{i=1}^{k} (\xi_i + \xi_i') - \sum_{i=1}^{k} \lambda_i (\varepsilon + \xi_i - y_i + \langle w, x_i \rangle + b) - \sum_{i=1}^{k} \eta_i (\varepsilon + \xi_i' + y_i - \langle w, x_i \rangle - b) - \sum_{i=1}^{k} (\eta_i \xi_i + \eta_i' \xi_i')
\] (8)

The solution of this optimization problem can be obtained by locating the saddle point of the Lagrange function defined in equation (8). The Saddle points of equation (8) can be obtained by equating partial derivative of \( L \) with respect to \( w, b, \xi_i \) and \( \xi_i' \) to zero. Thus, equation (5) can now be written as:

\[
f(x, \alpha) = \sum_{i=1}^{k} (\lambda_i' - \lambda_i) \langle x_i, x \rangle + b
\] (9)

The technique discussed above can be extended to allow for non-linear support vector regression by introducing the concept of the kernel function (Vapnik, 1995). 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 \( x_i \cdot x_j \) in equation (9) with \( \Phi(x_i) \cdot \Phi(x_j) \), where \( \Phi(x) \) is the mapping to the feature space; where \( K(x_i, x_j) \equiv \Phi(x_i) \cdot \Phi(x_j) \). Regression function given in equation (9) can now be written as:

\[
f(x, \alpha) = \sum_{i=1}^{k} (\lambda_i' - \lambda_i) K(x_i, x) + b
\] (10)

2.3 Gaussian Process

The Gaussian processes (GP) regression models are based on the assumption that adjacent observations should convey information about each other. They specify a prior directly over function space. This is a natural generalization of the Gaussian distribution whose mean is a vector and covariance is a matrix. The Gaussian distribution is based over vectors, whereas
the Gaussian process is based over functions. Therefore, due to prior knowledge about the data and functional dependencies, validation process is not required for generalization and Gaussian process regression models are able to understand the predictive distribution corresponding to test input (Rasmussen and Williams, 2006).

A Gaussian process is defined as a collection of random variables, any finite number which has a joint multivariate Gaussian distribution. Let $\mathcal{X} \times \mathcal{Y}$ represent the domain of inputs and outputs respectively, from which $n$ pairs $(x_i, y_i)$ are drawn independently and distributed identically. For regression, assume that $y \subseteq \mathbb{R}$, then a Gaussian process on $\mathcal{X}$ is defined by a mean function $\mu : \mathcal{X} \rightarrow \mathbb{R}$ and covariance function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$.

The main assumption of Gaussian process regression is that $y$ is given by $y = f(x) + \xi$ where $\xi \sim N(0, \sigma^2)$. The symbol $\sim$ in statistics means sampling for. In Gaussian process 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 $\xi$ is normal independent and distributed identically with mean value as zero ($\mu(x)=0$), variance $\sigma^2$ and $f(x)$ is drawn from the Gaussian process on $\mathcal{X}$ specified by $k$. That is,
\begin{equation}
Y = (y_1, \ldots, y_n) \sim N(0, K + \sigma^2 I) \tag{11}
\end{equation}
where $K_{ij} = k(x_i, x_j)$ and $I$ is the identity matrix.

Since $y/X \sim N(0, K + \sigma^2 I)$ is normal, so is the conditional distribution of test labels given training and test data $p(y_i|y, X, x_*)$. Then, one has $Y_*|Y, X, x_* \sim N(\mu, \Sigma)$ where
\begin{align}
\mu &= k(X, X)\{k(X, X) + \sigma^2 I\}^{-1} y \tag{12} \\
\Sigma &= k(X, X) - \sigma^2 I - k(X, X)\{k(X, X) + \sigma^2 I\}^{-1} k(X, X) \tag{13}
\end{align}
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 $y_j$, whereas $X_*$ is the vector of test data.

A specified covariance function is required to generate a positive semi-definite covariance matrix $K$, when $K_{ij} = k(x_i, x_j)$. The term kernel function used in support vector machines is equivalent to the covariance function used in Gaussian process regression. With the known values of kernel $k$ and degree of noise $\sigma^2$, equations (12) and (13) would be enough for inference.

During the training process of Gaussian Process regression models, one needs to choose a suitable covariance function as well as its parameters. In case of Gaussian process regression with a fixed value of Gaussian noise, the model can be trained by applying Bayesian inference, that is maximizing marginal likelihood. This leads to the minimization of the negative log-posterior:
\begin{equation}
p(\sigma^2, k) = \frac{1}{2} y^T \{K + \sigma^2 I\}^{-1} y + \frac{1}{2} \log \left| K + \sigma^2 I \right| - \log p(\sigma^2) - \log p(k) \tag{14}
\end{equation}
To find the hyper-parameters, the partial derivative of (14) can be obtained with respect to $\sigma^2$ and $k$ and minimization can be achieved by gradient descent. For further details about Gaussian process regression and different covariance function readers are referred to (Kuss, 2006).

3. Data Set

Data used in the present study are taken from an earlier study by Deswal (2008). The study has reported that oblique plunging jets ($\theta=60^\circ$) are more efficient than vertical plunging jets ($\theta=90^\circ$), and multiple oblique jets have higher oxygen transfer rate and efficiency in comparison to a single jet under similar flow conditions. The study, as stated earlier, has also proposed an empirical relationship (equation 4) to predict the overall volumetric oxygen transfer coefficient by multiple oblique jets for a given configuration (in terms of $d_j$, $v_j$ and $n$) under required flow conditions. The dataset consists of forty four experimental observations on different configurations of multiple oblique jets oxygenation system having jet impact angle of $60^\circ$. To predict the overall volumetric oxygen transfer coefficient ($K_{L,a(20)}$) by multiple oblique jets, three input parameters, namely $v_j$ (in m/s), $d_j$ (in m) and $n$ have been used. A ten-fold cross-validation has been 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 (Pal and Mather, 2003; Gill et al., 2006; Pal, 2006; Pal and Goel, 2006; Deswal and Verma, 2008; Pal and Deswal, 2008), and thus used in this study. In order to have a uniform comparison, RBF kernel has been used in GP regression as well. The optimal values of various user-defined parameters for neural network, support vector machines and Gaussian process are provided in Table 1.

<table>
<thead>
<tr>
<th>Approach</th>
<th>User defined parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neural network</td>
<td>Learning rate = 0.25, momentum = 0.2, Iterations =1000, Hidden layer = 1, hidden node = 8</td>
</tr>
<tr>
<td>Support vector machines</td>
<td>RBF kernel, $C = 20$, gamma = 2</td>
</tr>
<tr>
<td>Gaussian Process</td>
<td>RBF kernel, gamma = 1.2, noise = 0.1</td>
</tr>
</tbody>
</table>

4. Results

The values of overall oxygen transfer coefficient ($K_{L,a(20)}$) by multiple oblique jets have been estimated using neural network, SVMs and Gaussian process from the dataset for comparison. The three statistical parameters, namely correlation coefficient, coefficient of determination ($R^2$) and root mean square error (rmse) have been used to compare the relative performances of the computational techniques and with the empirical relationship of Deswal (2008) represented by equation (4).
Table 2: Statistical parameters.

<table>
<thead>
<tr>
<th>Approach</th>
<th>Correlation Coefficient</th>
<th>Root mean square error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neural network</td>
<td>0.982</td>
<td>0.002</td>
</tr>
<tr>
<td>Support vector machines</td>
<td>0.985</td>
<td>0.002</td>
</tr>
<tr>
<td>Gaussian Process</td>
<td>0.975</td>
<td>0.003</td>
</tr>
<tr>
<td>Equation (4)</td>
<td>0.981</td>
<td>0.002</td>
</tr>
</tbody>
</table>

Table 2 provides values of correlation coefficient and rmse values obtained using different approaches, that is the computational techniques and empirical relationship represented by equation (4). In general, all the three computational techniques have achieved statistically excellent correlation coefficient and root mean square error in predicting overall volumetric oxygen transfer coefficient \( K \alpha_{(20)} \) by multiple oblique jets oxygenation system. Statistically, the best results are obtained by SVM approach (corr. Coeff. = 0.985 and rmse = 0.002) followed by NN approach (corr. Coeff. = 0.982 and rmse = 0.002) and GP approach (corr. Coeff. = 0.975 and rmse = 0.003). When these results are compared with the empirical relationship (corr. Coeff. = 0.981 and rmse = 0.002), it has been revealed that the SVM and NN techniques have out-performed equation (4); however, GP technique could not out-perform but competitive with equation (4). Thus, suggesting the utility of all the above stated computational techniques for such environmental engineering applications.

Fig. 1 to Fig. 4 provide the graphs plotted between experimental and predicted values of overall volumetric oxygen transfer coefficient \( K \alpha_{(20)} \) at standard conditions by multiple oblique jets oxygenation system using NN, SVMs, GP and empirical relationship represented by equation (4) respectively. The plots depict the linear trend line of the data, line of perfect agreement between the experimental and predicted values, lines of ± 10 percent variation and coefficient of determination \( (R^2) \). The analysis revealed that SVMs and GP approaches along with equation (4) have predicted lower \( K \alpha_{(20)} \) values than the experimental values as is evident from the linear trend lines having lower inclination with respect to the line of perfect agreement. In case of neural network approach, the linear trend line is almost in agreement with the line of perfect agreement. This may lead to the inference that NN approach performs better than SVM approach, which is contrary to earlier statistical analysis (Table 1). A critical examination of Fig. 1 and Fig. 2 reveals that scattering of data (beyond ± 10 percent variation) is higher in case of NN than SVMs; but due to fairly equal counteracting (±) scattering in NN results, the trend line approaches the line of perfect agreement. So, it can now be safely pointed out that the performance of SVM is better than NN in the analysis. This is further strengthened by highest value of coefficient of determination with SVMs approach \( (R^2 = 0.968) \) followed by NN approach \( (R^2 = 0.963) \), equation (4) approach \( (R^2 = 0.962) \) and GP approach \( (R^2 = 0.948) \).
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Figure 1: Predicted $K_{La(20)}$ by neural network versus experimental $K_{La(20)}$.

Figure 2: Predicted $K_{La(20)}$ by support vector machines versus experimental $K_{La(20)}$. 
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Figure 3: Predicted \( K_{La(20)} \) by Gaussian process versus experimental \( K_{La(20)} \).

Figure 4: Predicted \( K_{La(20)} \) by equation (4) versus experimental \( K_{La(20)} \).
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Figure 5: Variation in predicted $K_{La(20)}$ values by computational techniques and equation (4) in comparison to the experimental $K_{La(20)}$ values by multiple oblique jets oxygenation system.

The variation of experimental and predicted overall volumetric oxygen transfer coefficient ($K_{La(20)}$) by multiple oblique jets with the number of test data is depicted in Fig. 5. It is evident from this plot that predicted $K_{La(20)}$ values by SVMs approach and equation (4) are in good agreement with actual experimental values; whereas, that is not relatively so in case of NN and GP approaches as the predicted values by these approaches are deviating at some of the test data points. Thus, suggesting a better performance of SVMs in comparison to by equation (4) and other computational techniques used in this study.

5. Conclusion

This study has investigated the potential of computational techniques in predicting overall volumetric oxygen transfer coefficient by multiple oblique jets oxygenation system in comparison with the empirical relationship suggested by Deswal (2008). The results presented are quite encouraging and recommends the application of support vector machines, neural network and Gaussian process regression techniques for analysing plunging jet oxygenation systems. Out of the three computational techniques, the performance of support vector machines was the best followed by neural network. The performance of support vector machines was found to be better than the empirical relationship in predicting the overall volumetric oxygen transfer coefficient by multiple oblique jets oxygenation system. Further, the application of support vector machines and neural network to such data set can be utilized in comparing the performance of single and multiple plunging jets of different configurations and also in designing and deciding the optimum configuration of multiple plunging jets for an efficient oxygenation system for given flow conditions.
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