Assessment of surface water quality is important in the management of water resources (Dogan et al. 2009). Water quality in rivers is paramount to the well-being of nature and humans, and surface water quality is usually related to the type of surrounding industries, agriculture, and human activities. Water is withdrawn from the hydrologic cycle to meet various needs and then is returned (Banejad & Olyaie 2011). Given the essential role of rivers to agricultural, industrial, and urban needs, it is necessary to regularly monitor and evaluate water quality in rivers. As rivers pass through different regions, changes in water quality and the level of hydrochemical parameters are observed in these regions. Because of the gradual decline in water quality over time, regulatory bodies in various countries have made decisions to mitigate the damage. Ecologically acceptable water management calls for accurate modeling, forecasting, and analyzing water quality in rivers (Durdu 2010). Numerous models have been developed for management of water quality, such as QUAL2E, Water Quality Analysis Simulation, and the US Army Corps of Engineers’ Hydrologic Engineering Center-5Q (Chen et al. 2003). Using these models is time-consuming and expensive; therefore, development of cost-effective models is encouraged.

Because of the propensity of varied standards for water quality, different parameters are used as quality indicators. The quantity of ammonia, cadmium, chemical oxygen demand, chlorine, copper, dissolved phosphorus, lead, nitrogen dioxide, suspended solids, total nitrogen, total phosphorus, zinc, sodium, sodium adsorption ratio, sulfate ions, bicarbonate ions, electrical conductivity (EC), total dissolved solids (TDS), and pH is frequently measured at water quality monitoring stations. EC and TDS levels in water are two of the main parameters used to determine quality of drinking and agricultural water because they directly represent the total concentration of salt in water. High EC and TDS values are not desirable in water used for irrigation because salt affects plant growth through osmosis (Phocaides 2000).

Advances in data science and data mining methods such as neural networks (NNs), fuzzy inference methods, support vector machines (SVMs), and k-nearest neighbors (k-NN), have made it possible to solve complex problems in high dimensions. The general principle behind these methods lies in exploring hidden relationships in large volumes of data and building models that reflect physical processes governing the system under study. A data-derived model represents a relationship between input variables and output variables. Such a model can be highly accurate because it captures relationships of any kind that are expressed in data, including the underlying physics and chemistry.

**DATA SCIENCE METHODS**

The growing use of data science methods in water resources engineering is seen in recent literature. Diamantopoulou et al.
In addition, data science models have been found to be cost-effective and time-effective. Liao et al. (2012) assessed water quality using an SVM and a genetic algorithm. They concluded that these algorithms provided acceptable results for estimating a variety of metal contaminants and were also effective in classifying water quality. Abbasi et al. (2013) proposed an NN model to predict changes in TDS in groundwater in Tehran Plain. They concluded that sulfate and chloride ions were more appropriate than sodium ions to model an NN. Heydari et al. (2013) developed an NN model to predict water quality parameters in the Delaware River in Pennsylvania, U.S. Li et al. (2013) used an SVM to measure the quality of surface water in Taihu Tiaoxi Lake, China. They found that the SVM model accurately classified water quality. Nikoo and Mahjouri (2013) studied water quality zoning based on the Water Quality Index (WQI) in both surface water and groundwater quality using probabilistic SVMs as well as self-organizing maps; they validated the efficiency of these methods. Saghebian et al. (2013) classified the quality of groundwater using a decision tree approach in Ardebil Plain, Iran. They observed that this method was effective in predicting water quality categories that are based on the US Salinity Laboratory diagram. Liu and Lu (2014) predicted water quality of rivers by estimating total nitrogen and total phosphorus using SVM and NN approaches and observed that SVMs provided higher accuracy results.

New models involving chemical parameters of river water have been developed and the accuracy of predicting EC and TDS values has been reported. The models proposed in this study offer a virtual alternative to hardware sensors. Data-driven models can be used to validate sensory measurements (this is important in condition monitoring) or as a replacement for some of the existing sensors (digital sensors tend to be accurate). On the other hand, it is known that directly and indirectly measuring EC and TDS values is expensive in Iran. Therefore, development of a model with a minimal number of chemical parameters but with acceptable accuracy to estimate EC and TDS values reduces the cost of water quality monitoring. Various data-mining algorithms have been applied to analyze data. The support vector regression (SVR) and k-NN algorithms have been found to provide the most accurate predictions of water parameters because of their inherent ability to handle the nonlinearity hidden in data of the phenomena studied in this research. This study aimed to estimate EC and TDS quality parameters in the Lighvan Chay River, Eastern Azerbaijan, Iran, using the SVR and k-NN methods.

**MATERIALS AND METHODS**

**Area studied and data used.** The area under study is the Lighvan Chay River located in the northern slopes of Mount Sahand, Iran. Hydrochemical data collected from the Lighvan hydrometric station between 1967 and 2011 were used to evaluate and predict TDS and EC of the Lighvan Chay River. The Lighvan station is located at latitude 38°9' north and longitude 46°24' east. This station is 1,450 m above the free water surface. Figure 1 shows the area under study with the rivers and Lighvan Hydrometric Station locations.

In this study, the effectiveness of hydrochemical parameters and the quantity of sodium adsorption ratio, pH, chlorine,
calcium (Ca), sulfate, bicarbonate, magnesium (Mg), and sodium are studied to predict values of EC and TDS. The range of parameters affecting water quality and their basic statistics are presented in Table 1.

The data set used in this research was obtained from the Regional Water Authority of Eastern Azerbaijan Province. In total, 433 data samples collected at the Lighvan station were used, of which 286 (66% of the data) were used for training and 147 (34%) were used for testing. In this research, river flow is not considered as an input parameter; therefore, data sets were arranged randomly at the preprocessing phase because of independent sampling time and data uniformity. Different combinations of hydrochemical parameters were considered as inputs to the model and the impact of different hydrochemical parameters on the TDS and EC values was evaluated. The correlation matrix among the water quality parameters is presented in Table 2.

The values presented in Table 2 indicate that the TDS parameter of water is highly correlated with EC, chloride sodium, and bicarbonate ion. EC is also highly correlated with chlorine, bicarbonate ion, sodium, and Mg. Performance of the SVR and the k-NN models was examined using the correlation coefficient \( R \) in Eq 1, root mean square error (RMSE) in Eq 2, and mean absolute error (MAE) in Eq 3.

\[
R = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \bar{x})^2 \sum_{i=1}^{n} (y_i - \bar{y})^2}} \quad (1)
\]

\[
RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (x_i - y_i)^2} \quad (2)
\]

\[
MAE = \frac{1}{n} \sum_{i=1}^{n} |x_i - y_i| \quad (3)
\]

where \( \Sigma \) is the sum, \( x \) is the observed value, and \( y \) denotes the computed value.

**SVR.** SVMs are learning algorithms based on statistical learning theory (Vapnik 1995). SVMs have been developed for regression.

---

**TABLE 1** Range and statistics of Lighvan (Eastern Azerbaijan, Iran) station data

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Minimum</th>
<th>Maximum</th>
<th>Mean</th>
<th>SD</th>
</tr>
</thead>
<tbody>
<tr>
<td>TDS</td>
<td>mg/L</td>
<td>62</td>
<td>1,573</td>
<td>190.055</td>
<td>99.343</td>
</tr>
<tr>
<td>EC</td>
<td>µS/cm</td>
<td>100</td>
<td>2,420</td>
<td>295.801</td>
<td>151.939</td>
</tr>
<tr>
<td>Ph</td>
<td>—</td>
<td>6.2</td>
<td>10.3</td>
<td>7.575</td>
<td>0.613</td>
</tr>
<tr>
<td>Cl</td>
<td>mg/L</td>
<td>0.1</td>
<td>11.25</td>
<td>0.665</td>
<td>0.74</td>
</tr>
<tr>
<td>Ca</td>
<td>mg/L</td>
<td>0.4</td>
<td>6.8</td>
<td>1.264</td>
<td>0.503</td>
</tr>
<tr>
<td>Mg</td>
<td>mg/L</td>
<td>0.04</td>
<td>10.2</td>
<td>0.589</td>
<td>0.582</td>
</tr>
<tr>
<td>Na</td>
<td>mg/L</td>
<td>0.05</td>
<td>10.2</td>
<td>1.122</td>
<td>0.735</td>
</tr>
<tr>
<td>SAR</td>
<td>mg/L</td>
<td>0.058</td>
<td>7.323</td>
<td>1.193</td>
<td>0.695</td>
</tr>
<tr>
<td>SO(_4^\text{2-})</td>
<td>mg/L</td>
<td>0.02</td>
<td>4.2</td>
<td>0.442</td>
<td>0.415</td>
</tr>
<tr>
<td>HCO(_3^\text{2-})</td>
<td>mg/L</td>
<td>0.2</td>
<td>11.1</td>
<td>1.866</td>
<td>0.784</td>
</tr>
</tbody>
</table>

**TABLE 2** Correlation matrix among water quality parameters

<table>
<thead>
<tr>
<th></th>
<th>SAR</th>
<th>Na</th>
<th>Mg</th>
<th>Ca</th>
<th>SO(_4^\text{2-})</th>
<th>Cl</th>
<th>HCO(_3^\text{2-})</th>
<th>Ph</th>
<th>EC</th>
<th>TDS</th>
</tr>
</thead>
<tbody>
<tr>
<td>SAR</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Na</td>
<td>0.87</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mg</td>
<td>0.01</td>
<td>0.37</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ca</td>
<td>0.01</td>
<td>0.36</td>
<td>0.53</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SO(_4^\text{2-})</td>
<td>0.39</td>
<td>0.43</td>
<td>0.23</td>
<td>0.32</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cl</td>
<td>0.46</td>
<td>0.79</td>
<td>0.66</td>
<td>0.57</td>
<td>0.20</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HCO(_3^\text{2-})</td>
<td>0.19</td>
<td>0.49</td>
<td>0.71</td>
<td>0.71</td>
<td>0.05</td>
<td>0.56</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ph</td>
<td>-0.13</td>
<td>-0.08</td>
<td>0.06</td>
<td>-0.01</td>
<td>0.01</td>
<td>-0.05</td>
<td>-0.13</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EC</td>
<td>0.44</td>
<td>0.76</td>
<td>0.75</td>
<td>0.73</td>
<td>0.41</td>
<td>0.83</td>
<td>0.78</td>
<td>-0.01</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>TDS</td>
<td>0.43</td>
<td>0.76</td>
<td>0.74</td>
<td>0.73</td>
<td>0.41</td>
<td>0.83</td>
<td>0.78</td>
<td>-0.02</td>
<td>0.99</td>
<td>1</td>
</tr>
</tbody>
</table>

Ca—calcium, Cl—chlorine, EC—electrical conductivity, HCO\(_3^\text{2-}\)—bicarbonate ion, Mg—magnesium, Na—sodium, Ph—phosphorus, SAR—sodium adsorption ratio, SD—standard deviation, SO\(_4^\text{2-}\)—sulfate, TDS—total dissolved solids.
called SVR, to estimate real value functions. In this case, the aim of learning is to find a function \(f(x)\) approximating the function \(y(x)\) with minimum risk, using the available independent and identically distributed data (Behzad et al. 2009).

\[
(x_1, y_1), \ldots, (x_m, y_m) \subseteq (X \subseteq \mathbb{R}^n \times Y \subseteq \mathbb{R})
\]  

The SVR algorithm estimates are based on a subset of training samples, called support vectors (Behzad et al. 2009). A loss function, presented in Eq 5 and called \(\varepsilon\)-insensitive loss, is used to induce sparseness \(R_e\).

\[
|y - f(x)|_\varepsilon = \begin{cases} 
0 & \text{if } |y - f(x)| \leq \varepsilon \\
|y - f(x)| - \varepsilon & \text{otherwise}
\end{cases}
\]  

where \(f(x)\) is computed by the SVR and estimates \(y\), and \(\varepsilon\) is the error.

The regression algorithm begins with the linear function estimation. Every linear function of input vector \(x\) has the representation in Eq 6:

\[
f(x) = (w; x) + b, \text{ where } w, x \in \mathbb{R}^n, b \in \mathbb{R}
\]

Note that in Eq 6, \((w, x)\) indicates the inner product of two vectors in the Hilbert space (i.e., a space in which the inner product of two vectors has a real value, also called inner or dot product space). To find \(f(x)\), one should minimize the regulated risk functional \((R_{reg})\) (instead of only empirical risk function used in traditional learning algorithms, such as NNs) defined in Eq 7.

\[
R_{reg}|f| = \frac{1}{2} \|w\|^2 + C R_{emp}|f|
\]

where \(R_{emp}|f| = \frac{1}{m} \sum_{i=1}^{m} |y_i - f(x_i)|_\varepsilon\)

The \(k\)-NN algorithm. The \(k\)-NN is a nonparametric method used for classification and regression. The input consists of the \(k\) closest training examples in the feature space. The output depends on whether \(k\)-NN is used for classification or regression. In the \(k\)-NN regression, output is the average of the values of its \(k\)-NN. The \(k\)-NN regression algorithm computes a weighted average of the \(k\)-NNs, which are weighted by the inverse of their distance. The algorithm computes a distance between the query example and the labeled examples and orders the labeled examples in increasing distance. Then heuristically \(k\)-NNs are determined on the basis of RMSE. A case is classified by a majority vote of its neighbors, with the case being assigned to the class most common among its \(k\)-NN measured by a function. If \(k = 1\), then the case is simply assigned to the class of its nearest neighbor (Larose 2004). In this study, open-source WEKA software (www.cs.waikato.ac.nz/ml/weka/) was used for SVR and \(k\)-NN modeling.

RESULTS AND DISCUSSION

EC is highly correlated to TDS; thus, accurate estimation of the amount of EC in water is an important step in obtaining an accurate estimate of TDS. TDS and EC of the water were obtained using the \(k\)-NN algorithm. The best number of neighbors was determined to be five by a trial-and-error approach. It was also observed that the Manhattan function performed best among the various distance functions considered. Several scenarios involving different input parameters, different neighbors, and various distance functions of the \(k\)-NN algorithm and different kernel functions of SVR were defined to obtain the most accurate estimates of EC and TDS (Tables 3 and 4). Then the best values of these parameters were selected. Various kernel functions of SVR were tested in modeling EC and TDS. It was determined that the radial basis function performed best in modeling TDS and EC among different kernel functions, such as linear function, polynomial functions, radial basis function, and sigmoid function. Tables 3 and 4 present different combinations of parameters for estimation of EC and TDS.

On the basis of the data in Tables 3 and 4, the accuracy (measured by \(R\)) of the models derived by the two algorithms is similar. The accuracy of these algorithms in handling different scenarios was also assessed. The data in Tables 3 and 4 indicate that scenario 3 offers the better quality estimates of TDS and EC than the remaining scenarios do. This scenario includes the input parameters of sodium, Mg, Ca, chloride, and bicarbonate ion, which highly affect the estimated values of EC and TDS. In Table 2, correlation between chemical parameters is reported. The selection of scenarios and combinations is based on the results in Table 2. The parameters in scenario 3 better correlate with target parameters (EC and TDS). The computational results demonstrate that selecting water quality hydrochemical parameters as inputs based on a correlation matrix was useful. Considering EC as an input parameter has increased the accuracy of the TDS estimation; this agrees with the direct relationship between EC and TDS. However, because field measurements of EC are as costly as field measurements of TDS, EC was not considered as the main parameter. The former provides less accurate results with fewer input parameters. Figures 2 and 3 illustrate the average value of the absolute error for different scenarios in the \(k\)-NN and SVR methods.

In Figures 2 and 3, the mean absolute error in the model selection \(R_s\) was used. In this study, the \(R\) criteria showed that scenario 3 is the best. Also, the number of input parameters in each scenario is important. Models with a smaller number of parameters as inputs are preferred. As can be seen in Figures 2 and 3, the scenarios with fewer parameters result in a higher mean absolute error. This indicates sensitivity to the number of input parameters. It also can be observed that the scenarios with sodium, Ca, Mg, chloride, and bicarbonate ion parameters have led to accurate results. This indicates a close relationship between the value of these parameters and the amount of EC and TDS in water. It can
### TABLE 3  
EC estimation results for different scenarios by SVR and \( k \)-NN methods

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Input Parameters</th>
<th>SVR</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>MAE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \mu \text{S/cm} )</td>
</tr>
<tr>
<td>1</td>
<td>SAR, Na, Mg, Ca, Cl, Ph, SO(_4), HCO(_3)</td>
<td>14.82</td>
</tr>
<tr>
<td>2</td>
<td>SAR, Na, Mg, Ca, Cl, HCO(_3)</td>
<td>17.07</td>
</tr>
<tr>
<td>3</td>
<td>Na, Mg, Ca, Cl, HCO(_3)</td>
<td>16.97</td>
</tr>
<tr>
<td>4</td>
<td>Na, Ca, Cl, HCO(_3)</td>
<td>23.80</td>
</tr>
<tr>
<td>5</td>
<td>Na, Mg, Cl, HCO(_3)</td>
<td>23.61</td>
</tr>
<tr>
<td>6</td>
<td>Ca, Cl, HCO(_3)</td>
<td>27.21</td>
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<tr>
<td>7</td>
<td>Na, Ca, Cl, HCO(_3)</td>
<td>25.19</td>
</tr>
<tr>
<td>8</td>
<td>Cl, HCO(_3)</td>
<td>27.52</td>
</tr>
</tbody>
</table>

### TABLE 4  
TDS estimation results for different scenarios by SVR and \( k \)-NN methods

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Input Parameters</th>
<th>SVR</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>MAE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \text{mg/L} )</td>
</tr>
<tr>
<td>1</td>
<td>SAR, Na, Mg, Ca, Cl, Ph, SO(_4), HCO(_3)</td>
<td>10.96</td>
</tr>
<tr>
<td>2</td>
<td>SAR, Na, Mg, Ca, Cl, HCO(_3)</td>
<td>11.95</td>
</tr>
<tr>
<td>3</td>
<td>Na, Mg, Ca, Cl, HCO(_3)</td>
<td>11.90</td>
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<tr>
<td>4</td>
<td>Na, Ca, Cl, HCO(_3)</td>
<td>15.42</td>
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<td>5</td>
<td>Na, Mg, Cl, HCO(_3)</td>
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<td>6</td>
<td>Ca, Cl, HCO(_3)</td>
<td>17.59</td>
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<td>7</td>
<td>Na, Ca, Cl, HCO(_3)</td>
<td>15.93</td>
</tr>
<tr>
<td>8</td>
<td>Cl, HCO(_3)</td>
<td>18.18</td>
</tr>
</tbody>
</table>

Ca—calcium, Cl—chlorine, EC—electrical conductivity, HCO\(_3\)—bicarbonate ion, \( k \)-NN—\( k \)-nearest neighbors algorithm, MAE—mean absolute error, Mg—magnesium, Na—sodium, Ph—phosphorus, RMSE—root mean square error, SAR—sodium adsorption ratio, SO\(_4\)—sulfate, SVR—support vector regression

### FIGURE 2  
The mean absolute error for different scenarios of estimating electrical conductivity

### FIGURE 3  
The mean absolute error values for different scenarios of estimating total dissolved solids

Ca—calcium, Cl—chlorine, HCO\(_3\)—bicarbonate ion, \( k \)-NN—\( k \)-nearest neighbors algorithm, MAE—mean absolute error, Mg—magnesium, Na—sodium, Ph—phosphorus, RMSE—root mean square error, SAR—sodium adsorption ratio, SO\(_4\)—sulfate, SVR—support vector regression, TDS—total dissolved solids
FIGURE 4  Scatter diagram of SVR model for predicted and observed TDS values

\[ y = 0.8994x + 19.149 \]
\[ R^2 = 0.8345 \]

SVR—support vector regression, TDS—total dissolved solids

FIGURE 5  Scatter diagram of the k-nearest neighbors model for predicted and observed TDS values

\[ y = 0.8136x + 29.67 \]
\[ R^2 = 0.8035 \]

TDS—total dissolved solids

FIGURE 6  Comparison of the TDS results obtained from SVR and k-NN models with the observed values

FIGURE 7  Comparison of the EC results obtained from SVR and k-NN models with the observed values

FIGURE 8  Scatter diagram of support vector regression for predicted and observed values of EC

\[ y = 0.9066x + 26.427 \]
\[ R^2 = 0.8568 \]

EC—electrical conductivity

FIGURE 9  Scatter diagram of k-NN predicted and observed EC values

\[ y = 0.8251x + 44.254 \]
\[ R^2 = 0.8378 \]

EC—electrical conductivity, k-NN—k-nearest neighbors
also be observed that the SVR method generally produces smaller errors than the k-NN method. The observed and compared values of TDS and EC produced by the k-NN and SVR models are shown in Figures 4–7.

As can be seen in Figures 4, 5, 8, and 9, the SVR approach provides more accurate estimates of TDS and EC than the k-NN model. The computed values track the observed values. Both methods estimate EC more accurately than does TDS.

As can be seen in Figures 6 and 7, the SVR model offers greater flexibility to sudden changes in the values of EC and TDS than the k-NN model. This implies that the SVR model is more adaptive to sudden changes in these parameters.

CONCLUSION

The EC and TDS parameters are widely used to determine quality of drinking and agricultural water because they directly represent the total concentration of salt in water. This research was motivated by the need to determine an accurate and affordable method to predict EC and TDS, the available EC and TDS probes are not accurate because of the nonlinear relationship between EC and TDS. This research has demonstrated that TDS can be accurately predicted using only five parameters.

Another motivation for the research was to evaluate suitability of data-mining algorithms to model relationships between parameters of the river water. Data-driven models can be used to validate sensory measurements of traditional sensors. Also, this research has shown that the best scenario to estimate the TDS in water and EC involves a combination of the following parameters: sodium, Mg, Ca, chloride, and bicarbonate ion. Similar research (Abbasi et al. 2013) examined changes in TDS in the Tehran Plain groundwater using an NN model. Using sulfate, chloride, and sodium, in the best case the authors obtained an R of 0.96 with an RMSE of 175.15; the total mean error was 114.24. However, this report shows a higher R, lower RMSE, and smaller total error than those obtained in the study reported in Abbasi et al. 2013. The research discussed in this article reveals that SVR and k-NN methods can accurately predict TDS and EC values in the Lighvan Chay River. The SVR model is recommended because of better performance. The computational results show there was no need to use the costly process of sampling hydrochemical parameters that affect river water quality. Rather, using fewer hydrochemical parameters has led to acceptable accuracy in estimating TDS and EC values. The approach discussed in this article reduces the cost of the water quality monitoring.

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He has authored and coauthored approximately 50 national and international journal articles. In addition, he has undertaken five scientific projects in Iran and two in Turkey. Ali Rezaazadeh Jouidi is in the Young Researchers and Elite Club, Maragheh Branch, Islamic Azad University, Maragheh, Iran. Andrew Kusiak is a professor in the Department of Mechanical and Industrial Engineering, The University of Iowa, Iowa City.

REFERENCE


