Supporting Information

Minimization of electrical energy consumption in the photocatalytic reduction of Cr(VI) by using immobilized Mg, Ag co–impregnated TiO$_2$ nanoparticles

Hamed Eskandarloo $^a$, Alireza Badiel $^{a,*}$, Mohammad A. Behnajady $^b$, Ghodsi Mohammadi Ziarani $^c$

$^a$ School of Chemistry, College of Science, University of Tehran, Tehran, Iran

$^b$ Department of Chemistry, College of Science, Tabriz Branch, Islamic Azad University, Tabriz, Iran

$^c$ Department of Chemistry, Faculty of Science, Alzahra University, Tehran, Iran

*Corresponding author:

E–mail Address: abadiei@ut.ac.ir

Tel.: +98–2161112614; Fax: +98–2161113301
3.1. Model analysis

The mathematical relationship of the response on these variables can be approximated by second–order polynomial equation as shown below:

\[ Y = b_0 + b_1x_1 + b_2x_2 + b_3x_3 + b_{12}x_1x_2 + b_{13}x_1x_3 + b_{23}x_2x_3 + b_{11}x_1^2 + b_{22}x_2^2 + b_{33}x_3^2 \]  

(1)

where \( Y \) is a predicted response of photocatalytic reduction efficiency, \( b_0 \) is the constant, \( b_1, b_2, \) and \( b_3 \) are the regression coefficients for linear effects, \( b_{12}, b_{13}, \) and \( b_{23} \) are the regression coefficients for interaction effects, \( b_{11}, b_{22}, \) and \( b_{33} \) are the regression coefficients for squared effects and \( x_i \) is coded experimental levels of the Mg, Ag co–impregnated TiO\(_2\) synthesis variables.

Based on the results in Table 1, an empirical relationship between the response (\( Y \)) and independent synthesis variables (\( x_1, x_2, x_3 \), see Table S1) was attained as shown in Eq. (2):

\[ Y = 67.47 - 6.78x_1 + 7.79x_2 + 4.49x_3 - 2.41x_1x_2 - 6.65x_1x_3 - 3.80x_2x_3 - 3.35x_1^2 - 8.33x_2^2 - 9.68x_3^2 \]  

(2)

Equation (2) is used to predict the photocatalytic reduction of Cr(VI) by the Mg, Ag co–impregnated TiO\(_2\) nanoparticles in a fixed–bed system with varied synthesis variables within the selected experimental ranges. By using resulted second–order polynomial equation (Eq. (2)), the predicted values of photocatalytic reduction of Cr(VI) is plotted versus corresponding experimental results in Figure S1. The results confirm that the predicted photocatalytic reduction rate from the model is in good agreement with the experimental results.

Analysis of variance (ANOVA) of the quadratic response surface model is a statistical procedure to test the significance and adequacy of the model.\(^1\) Table S2 shows the ANOVA results for quadratic response surface model. According to the ANOVA results, the regression model present a high correlation coefficient (\( R^2 = 0.9635 \)) for the photocatalytic reduction of Cr(VI). The value
of $R^2$ implies a satisfactory representation of photocatalytic reduction process by the model. Adjusted $R^2$ is also used to measure the goodness of fit between model and experimental data. Adjusted $R^2$ value (0.9027) was close to the corresponding $R^2$ value. The $F$–value, is the ratio between the mean square of the model and the residual error, and indicates the significance of each controlled factor on the tested model. The $F$–value for the model is 13.22 and the corresponding $p$–value is $<0.0001$. These results indicated that the model was statistically significant and there is only a 0.01% chance that the “model $F$–value” could occur due to noise.
References:


Figure S1. Comparison between predicted and experimental reduction rate of Cr(VI) by Mg, Ag co–impregnated TiO$_2$ nanoparticles.

Figure S2. SEM micrograph of Mg, Ag co–impregnated TiO$_2$ nanoparticles immobilized nanoparticles on the glass plate, picture from the surface.
Table S1. Experimental ranges and levels of the synthesis variables.

<table>
<thead>
<tr>
<th>Synthesis variables</th>
<th>Symbol</th>
<th>Ranges and levels</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>( x_1 )</td>
</tr>
<tr>
<td>Mg concentration (wt%)</td>
<td>( x_1 )</td>
<td>(0)</td>
</tr>
<tr>
<td>Ag concentration (wt%)</td>
<td>( x_2 )</td>
<td>(0)</td>
</tr>
<tr>
<td>Calcination temperature (°C)</td>
<td>( x_3 )</td>
<td>(282)</td>
</tr>
</tbody>
</table>

Table S2. ANOVA results of the response surface quadratic model for the photocatalytic reduction of Cr(VI).

<table>
<thead>
<tr>
<th>Source of variations</th>
<th>Sum of squares</th>
<th>Degree of freedom</th>
<th>Mean square</th>
<th>(F)-Value</th>
<th>(p)-Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regression</td>
<td>4431.84</td>
<td>9</td>
<td>492.43</td>
<td>13.22</td>
<td>&lt; 0.0001</td>
</tr>
<tr>
<td>Residual</td>
<td>372.41</td>
<td>10</td>
<td>37.24</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>4804.25</td>
<td>19</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\(R^2 = 0.9635\), adjusted \(R^2 = 0.9027\).