Combined physico-chemical treatment of secondary settled municipal wastewater in a multifunctional reactor

SUPPLEMENTARY INFORMATION

Governing equations

All the flow and mass transfer equations are presented in Cartesian tensor notation. For a steady incompressible flow, the conservation laws of mass, momentum and concentration are written as:

Continuity:
\[ \frac{\partial U_j}{\partial x_j} = 0 \]  
(1)

Momentum:
\[ \frac{\partial (\rho U_j U_i)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \mu \frac{\partial U_j}{\partial x_j} - \rho \overline{u_i u_j} \right) \]  
(2)

Mass fraction:
\[ \frac{\partial (\rho U_j Y_i)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial Y_i}{\partial x_j} - \rho \overline{u_i u_j} Y_i \right) \]  
(3)

where \( U_j \) is the velocity component and \( x_j \) is Cartesian coordinate. In Equation (2) \( P \) is the pressure, \( \rho \) is the density, \( \mu \) is the dynamic viscosity, \( -\rho \overline{u_i u_j} \) is the unknown Reynolds tensor, while in Equation (3) \( Y_i \) represents the species mass fraction of \( i \)th component. The unknown \( -\rho \overline{u_i u_j} \) is the diffusion term of species due to the turbulent flow and \( Sc \) is the molecular Schmidt number.

In this study, the closure of the mean equations is based on Boussinesq’s hypothesis of eddy-viscosity. According to eddy-viscosity hypothesis, the Reynolds stress tensor, the Reynolds stress tensor, takes the form:
\[ -\rho \overline{u_i u_j} = \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \rho k \]  
(4)

where \( k \) is turbulent kinetic energy, and the turbulent viscosity, \( \mu_t \), is obtained from:
\[ \mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \]  
(5)

Similarly the scalar flux \(-\rho \overline{u_i u_j} Y_i\) is modeled through the eddy-diffusion hypothesis as:
\[ -\rho \overline{u_i u_j} Y_i = \frac{\mu_t}{Sc_T} \frac{\partial Y_i}{\partial x_j} \]  
(6)

where \( Sc_T \) is turbulent Schmidt number.

In this study, the standard \( k - \varepsilon \) model is used to obtain the turbulent viscosity. The standard \( k - \varepsilon \) model is a semi-empirical model based on model transport equations for the turbulent kinetic energy (\( k \)) and its dissipation rate (\( \varepsilon \)) which are obtained from the following transport equations:

\[ \frac{\partial (\rho u_j k)}{\partial x_j} = \rho P_k - \rho \varepsilon + \frac{\partial}{\partial x_j} \left[ \mu_t \frac{\partial k}{\partial x_j} \right] \]  
(7)

\[ \frac{\partial (\rho u_j \varepsilon)}{\partial x_j} = c_{\varepsilon 1} \rho \frac{\varepsilon P_k}{k} - c_{\varepsilon 2} \rho \varepsilon^2 \frac{k}{k} + \frac{\partial}{\partial x_j} \left[ \mu_t \frac{\partial \varepsilon}{\partial x_j} \right] \]  
(8)

In the above equations \( P_k \) is the generation rate of turbulent kinetic energy obtained from:
\[ P_k = \nu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \]  
(9)

All constants appearing in Equations (5)–(8) are given in Table S1.

<table>
<thead>
<tr>
<th>( C_\varepsilon )</th>
<th>( C_{\varepsilon 1} )</th>
<th>( C_{\varepsilon 2} )</th>
<th>( \sigma_\varepsilon )</th>
<th>( \sigma_\varepsilon )</th>
<th>( Sc_T )</th>
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<td>1.92</td>
<td>1.0</td>
<td>1.3</td>
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Table S1 | Empirical constants of the \( k - \varepsilon \) turbulence model