Estimating soil specific surface area using the summation of the number of spherical particles and geometric mean particle-size diameter

Hamid Reza Fooladmand

Department of Irrigation, Marvdasht Branch, Islamic Azad University, Marvdasht, Iran. E-mail: hrfoolad@yahoo.com.

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Soil specific surface area (SSA) is an important soil property. SSA can be estimated from soil textural data or soil particle-size distribution. In this study, 20 soils with appropriate combination of texture were selected from Fars province, south of Iran. For each soil sample the values of SSA and percentages of clay, silt and sand were measured. Also, soil particle-size distribution curve of each soil was estimated with an existing modified model, and then the summation of the number of spherical particles for whole parts of the soil particle-size distribution (N) was determined. Furthermore, the geometric mean particle-size diameter ($d_g$) of each soil was determined. Then, two power equations based on $d_g$ and N were calibrated to estimate SSA, and then the derived equations were validated for two independent soil data sets including 64 soils. Root mean square error (RMSE) was used to evaluate the obtained results in calibration and validation stages. The RMSE values of power equations based on $d_g$ and N in calibration stage equaled 76.3 and 91.3, respectively, and in validation stage equaled 97.4 and 57.1, respectively. Therefore, the power equation based on $d_g$ was better than the power equation based on N for estimating SSA in calibration stage; however, the power equation based on N was better than the power equation based on $d_g$ for estimating SSA in validation stage.

Key words: Soil specific surface area, geometric mean particle-size diameter, summation of the number of spherical particles.

INTRODUCTION

The soil specific surface area (SSA) is defined as the sum of the surface area of soil particles per unit mass, and largely determines many physical and chemical properties of soil (Sepaskhah et al., 2010). SSA influences soil quality, and many phenomena such as adsorption of molecules, heat loss or grain resulting from adsorption, swelling and shrinkage, and many other physical and chemical processes are closely related to SSA (Petersen et al., 1996). Hillel (1980) indicates that the measurements of SSA are more meaningful and pertinent index for characterizing a soil than the percentages of clay, silt and sand. Since, SSA is highly dependent on soil texture, it may be successfully estimated from the soil textural data and soil particle-size distribution using fractal dimension (Ersahin et al., 2006) or simple regression equations. In many studies, a significant positive relationship between SSA with clay content, and negative relationship between SSA with sand content have been reported (Ratner-Zohar et al., 1983; Puckett et al., 1985; Ben-Dor and Banin, 1995; Petersen et al., 1996; Or and Tuller, 1999; Ersahin et al., 2006; Hepper et al., 2006).

Different methods have been presented to measure the value of SSA. Many investigators used ethylene glycol monoethyle ether (EGME) to measure SSA (Cerato, 2002; Ersahin et al., 2006; Fooladmand and Kaveh, 2010). However, this method is time-consuming and laborious; therefore, an estimation of SSA is preferred (Sepaskhah et al., 2010). As mentioned before, due to the highly dependence of SSA on soil texture, it can be successfully estimated from the soil textural data and soil particle-size distribution. Shirazi and Boersma (1984) proposed the geometric mean particle-size diameter based on the values of clay, silt and sand contents, and Sepaskhah et al. (2010) estimated SSA based on this soil property. On the other hand, Fooladmand (2008) estimated soil cation exchange capacity based on soil organic matter content, soil textural data, geometric mean particle-size diameter, and the summation of the number of spherical particles for whole parts of the soil particle-
size distribution. Therefore, the objective of this study was to estimate SSA based on the geometric mean particle-size diameter and the summation of the number of spherical particles for whole parts of the soil particle-size distribution. Up to now, the value of summation of the number of spherical particles for whole parts of the soil particle-size distribution has not been used for estimating SSA. However, in this study the role of this soil property for estimating SSA have been investigated, and the results have been compared with estimating SSA based on the geometric mean particle-size diameter of each soil.

MATERIALS AND METHODS

For this study, 20 soils in cultivated field were selected from different locations in Fars province, south of Iran. The soil samples have been selected to acheive an appropriate combination of soil texture. The clays of all selected soils have similar mineralogy, so that the majority of the selected soils was derived from alluvium, and all samples were taken from the topsoils (A horizons). For each soil, SSA was measured by ethylene glycol monoethyl ether (EGME) method as follows (Carter et al., 1986):

\[
SSA = \frac{W_a}{0.000286 W_s}
\]

(1)

where SSA is in m\(^2\)g\(^{-1}\), \(W_a\) is the mass of remained EGME in soil sample (g), and \(W_s\) is the mass of initial dry soil sample (g).

Also, the percentages of clay, silt and sand of each soil according to the USDA system for particle-size range (Clay: 0-0.002 mm; Silt: 0.002-0.05 mm; sand: 0.05-2 mm) were measured with a combination of the hydrometer and the wet sieving methods (Gee and Bauder, 1986). Then, the geometric mean particle-size diameter of each soil was calculated as follows (Shirazi and Boersma, 1984):

\[
d_g = \exp(f_c \ln M_c + f_{si} \ln M_{si} + f_{sa} \ln M_{sa})
\]

(2)

where \(d_g\) is the geometric mean particle-size diameter (mm), \(f_c\), \(f_{si}\) and \(f_{sa}\) are the clay, silt and sand fractions of soil (g g\(^{-1}\)), respectively, and \(M_c\), \(M_{si}\) and \(M_{sa}\) are the mean values diameter of clay, silt and sand, respectively (\(M_c = 0.001\) mm; \(M_{si} = 0.026\) mm; \(M_{sa} = 1.025\) mm).

Furthermore, soil particle-size distribution curve of each soil was estimated based on the percentages of clay, silt and sand. To do this, the proposed model by Skaggs et al. (2001) which has been modified by Fooladmand and Sepaskhah (2006) was used according to following equations:

\[
\alpha = -\frac{1}{\ln \frac{r_2 - r_0}{r_1 - r_0}}
\]

(3)

\[
\beta = \alpha \ln \frac{r_1 - r_0}{r_0}
\]

(4)

\[
v = \ln \frac{(cl + si)^{-1} - 1}{cl^{-1} - 1}
\]

(5)

\[
w = \ln \frac{(cl + si + sa)^{-1} - 1}{cl^{-1} - 1}
\]

(6)

\[
c = \alpha \ln \frac{v}{w}
\]

(7)

\[
u = \frac{(-v)^{1-\beta}}{(-w)^{-\beta}}
\]

(8)

\[
P = \frac{1}{1 + (cl^{-1} - 1) \exp\{-u(R - 1)^c\}}
\]

(9)

where \(r_0\), \(r_1\) and \(r_2\) equal to 1, 25 and 999 \(\mu m\), respectively, \(cl\), \(si\) and \(sa\) are the values of clay, silt and sand fractions (g g\(^{-1}\)), respectively, \(P\) is the mass fraction of soil particles (g g\(^{-1}\)) less than radius \(R\) (1 \(\mu m < R < 1000\) \(\mu m\)).

This model was used for nineteen proposed radii of 1, 1.5, 2.5, 5, 10, 15, 20, 25, 35, 50, 75, 100, 150, 200, 300, 400, 500, 750 and 1000 \(\mu m\) as reported by Fooladmand and Sepaskhah (2006). Also, the adjusted coefficients were used for radii of 1, 1.5, 2.5, 5, 10, 15 and 20 \(\mu m\) for soils with less than 60% silt or more than 60% silt as reported by Fooladmand and Sepaskhah (2006).

Arya and Paris (1981) and Arya et al. (1999) derived the following equation for determining the number of spherical particles for each fraction of the soil particle-size distribution:

\[
n_i = \frac{3P_i}{4\pi \rho_s R_i^3}
\]

(10)

where \(n_i\) is the number of spherical particles for each fraction of the soil particle-size distribution, \(R_i\) is the mean particle radius (cm) for the \(i\)th particle-size fraction, \(P_i\) is the fraction solid mass (g g\(^{-1}\)) and \(\rho_s\) is the soil particle density (g cm\(^{-3}\)).

The mass fraction of soil particles (\(P_i\)) for each soil particle radius (\(R_i\)) can be estimated by using the Equations (3) to (9). Then, the number of spherical particles for each fraction of the soil particle-size distribution was estimated by using the Equation (9) by converting the mentioned nineteen soil particle radii into cm. Also, the particle density of each soil was determined as follows:

\[
\rho_s = \frac{\rho_b}{1 - \theta_s}
\]

(11)

where \(\rho_b\) is the soil bulk density (g cm\(^{-3}\)), and \(\theta_s\) is the saturated volumetric soil water content (m\(^3\) m\(^{-3}\)).

Then, the summation of \(n\) for whole parts of the soil particle-size distribution was calculated as follows:

\[
N = \sum n_i
\]

(12)
Table 1. The mean, maximum and minimum of physical properties of the soils used for calibration and validation stages.

<table>
<thead>
<tr>
<th>Statistic criteria</th>
<th>SSA (m² g⁻¹)</th>
<th>Clay (%)</th>
<th>Silt (%)</th>
<th>Sand (%)</th>
<th>dₙ (mm)</th>
<th>N</th>
<th>ρₛ (g cm⁻³)</th>
<th>θₛ (m³ m⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calibration data</td>
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</tr>
<tr>
<td>Maximum</td>
<td>343.4</td>
<td>46.0</td>
<td>62.0</td>
<td>80.0</td>
<td>0.431</td>
<td>5.216 × 10¹⁰</td>
<td>1.67</td>
<td>0.547</td>
</tr>
<tr>
<td>Minimum</td>
<td>8.0</td>
<td>4.0</td>
<td>16.0</td>
<td>4.0</td>
<td>0.007</td>
<td>3.791 × 10⁸</td>
<td>1.16</td>
<td>0.373</td>
</tr>
<tr>
<td>Mean</td>
<td>149.0</td>
<td>24.4</td>
<td>46.9</td>
<td>28.8</td>
<td>0.094</td>
<td>2.735 × 10¹⁰</td>
<td>1.37</td>
<td>0.459</td>
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<tr>
<td>Validation data</td>
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<td>(Ersahin et al., 2006)</td>
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<td></td>
</tr>
<tr>
<td>Maximum</td>
<td>523.5</td>
<td>73.0</td>
<td>60.0</td>
<td>68.0</td>
<td>0.269</td>
<td>6.611 × 10¹⁰***</td>
<td>1.67***</td>
<td></td>
</tr>
<tr>
<td>Minimum</td>
<td>20.6</td>
<td>5.0</td>
<td>15.0</td>
<td>5.0</td>
<td>0.003</td>
<td>5.147 × 10⁹  ***</td>
<td>1.16***</td>
<td></td>
</tr>
<tr>
<td>Mean</td>
<td>162.9</td>
<td>40.0</td>
<td>37.1</td>
<td>22.9</td>
<td>0.040</td>
<td>3.766 × 10¹⁰***</td>
<td>1.37***</td>
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</tr>
<tr>
<td>Validation data</td>
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<tr>
<td>(Puckett et al., 1985)</td>
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</tr>
<tr>
<td>Maximum</td>
<td>59.1</td>
<td>42.1</td>
<td>35.8</td>
<td>88.5</td>
<td>0.642</td>
<td>4.169 × 10¹⁰</td>
<td>1.86</td>
<td>0.441</td>
</tr>
<tr>
<td>Minimum</td>
<td>2.5</td>
<td>1.4</td>
<td>7.4</td>
<td>34.6</td>
<td>0.033</td>
<td>1.608 × 10⁹</td>
<td>1.47</td>
<td>0.253</td>
</tr>
<tr>
<td>Mean</td>
<td>35.7</td>
<td>22.0</td>
<td>18.4</td>
<td>59.6</td>
<td>0.168</td>
<td>2.142 × 10¹⁰</td>
<td>1.63</td>
<td>0.349</td>
</tr>
</tbody>
</table>

*** These data were not measured, and in this study soil particle density of these soils were assumed 2.65 g cm⁻³ for using in Equation (10).

where N is the summation of the number of spherical particles for whole parts of the soil particle-size distribution.

Arya and Paris (1981) and Arya et al. (1999) derived N value from the soil particle-size distribution to estimate the soil physical properties from the pore size and the number of pores; however, in this study N value has been used directly for estimating SSA to determine the role of it for estimating SSA.

Sepaskhah et al. (2010) derived a power equation based on dₙ for estimating SSA by using the mentioned 20 soils in Fars province, south of Iran as follows:

\[ SSA = 3.89dₙ^{-0.905} \]

where SSA is in m² g⁻¹, and dₙ is in mm.

Sepaskhah et al. (2010) validated the Equation (13) for estimating SSA for 22 different soils in Turkey (Ersahin et al., 2006), and the results showed the appropriateness of this equation for estimating SSA. However, in this study another power equation based on N value for estimating SSA was derived by using the same 20 soil samples in Fars province, south of Iran. Also, for evaluating the results, in addition to 22 soils in Turkey (Ersahin et al., 2006), 42 other soils (Puckett et al., 1985) have been used.

RESULTS AND DISCUSSION

The maximum, minimum and mean values of SSA, the percentages of clay, silt and sand, dₙ, N, soil bulk density and saturated volumetric soil water content of the used soil samples for calibration and validation stages are presented in Table 1. The best derived equation between SSA and N for calibration stage had power shape as follows:

\[ SSA = 1 \times 10^{-13} N^{1.437} R^2 = 0.84 \]  \hspace{1cm} (14)

As shown, the best derived equation for estimating SSA based on N value are similar to equation based on dₙ, that is, the Equation (13). However, the R² value of Equation (14) is lower than the R² value of Equation (13); so that Equations (13) and (14) describe 88 and 84% of the variability in SSA, respectively. Also, root mean square error (RMSE) was used as follows to evaluate the obtained results for SSA estimation:

\[ RMSE = \left( \frac{\sum((SSA_c - SSA_m)^2)}{M} \right)^{0.5} \]  \hspace{1cm} (15)

where SSA_c and SSA_m are the estimated and measured SSA in each soil and M is the number of soil data sets.

The best condition for estimating SSA will give smaller value of RMSE. The RMSE values of Equations (13) and (14) for calibration stage equaled 76.3 and 91.3, respectively. Therefore, the power equation based on dₙ was better than the power equation based on N for estimating SSA in calibration stage. Therefore, Equation (13) is superior to equation (14) for the estimation of SSA in calibration stage according to the RMSE and R² values. It indicates that the appropriateness of power equation based on dₙ which has been derived by Sepaskhah et al. (2010).

The RMSE values of Equations (13) and (14) for 22 soils of Ersahin et al. (2006) in validation stage equaled 165.4 and 59.2, respectively. Therefore, the power
equation based on N was better for estimating SSA for these soils; while, Sepaskhah et al. (2010) without using the N value reported that the power equation based on $d_g$ was appropriate for estimating SSA of these soils. On the other hand, the RMSE values of Equations (13) and (14) for 42 soils of Puckett et al. (1985) in validation stage equaled 10.9 and 56.0, respectively. Therefore, the power equation based on $d_g$ was better for estimating SSA for these soils. However, the RMSE values of Equations (13) and (14) equaled 97.4 and 57.1, respectively in validation stage while total 64 soils were considered. Figure 1 shows the scattering point of measured and estimated SSA based on the Equations (13) and (14) around line one: one for all soils used in

Figure 1. The scattering point around line one: one for estimating SSA for validation soils. (a) based on Equation 13 (b) based on Equation 14.
(validation stage. As shown in this Figure 1, the scattering point around line one: one in Equation (14) is better than Equation (13). Therefore, the power equation based on N is better for estimating SSA in validation stage, which is in contrast to the obtained results in calibration stage. Consequently, the results of this study showed that using the N value may be tended to improve the estimation of SSA. Therefore, the proposed equation by Arya and Paris (1981) and Arya et al. (1999) for estimating the soil physical properties from the pore size and the number of pores, can be useful for estimating SSA, and the N value of soil has an important role for estimating SSA. It indicates that in addition to shape and size of a soil particle, the amount of N determines SSA and influences the strength of the interaction between water and soil particles. Moreover, the value of SSA depends on grain size distribution, and grain size distribution can be shown in the value of N. Also, an increase of fine fractions of soil such as clay content tends to increase the amount of N, and consequently tends to increase SSA, which is in agreement with the positive power of Equation (14).

Conclusions

Two power equations were used for estimating soil specific surface area (SSA) based on the geometric mean particle-size diameter ($d_m$) and the summation of the number of spherical particles for whole parts of the soil particle-size distribution (N). These equations have been calibrated using 20 soil samples with different textures in south of Iran. To determine the value of N of each soil, the proposed equation by Arya and Paris (1981) and Arya et al. (1999) was used, and to do this at first the soil particle-size distribution curve was estimated with the modified model proposed by Fooladmand and Sepaskhah (2006). Also, two independent soil data sets including 64 soil samples were used to validate the derived equations for estimating SSA. The results in validation stage indicated that using the value of N tended to improve estimation of SSA. Therefore, in addition to shape and size of a soil particle, the amount of N has important role in the value of soil SSA, which is in accordance to the fact that the value of SSA depends on grain size distribution. Therefore, according to the obtained results it is possible to use the value of N for estimating SSA; however, it is proposed to test the obtained results of this study for a wider soil data sets at different locations of the world with different textures.

REFERENCES