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Grain-size model for hydraulic conductivity estimation of porous media

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ABSTRACT

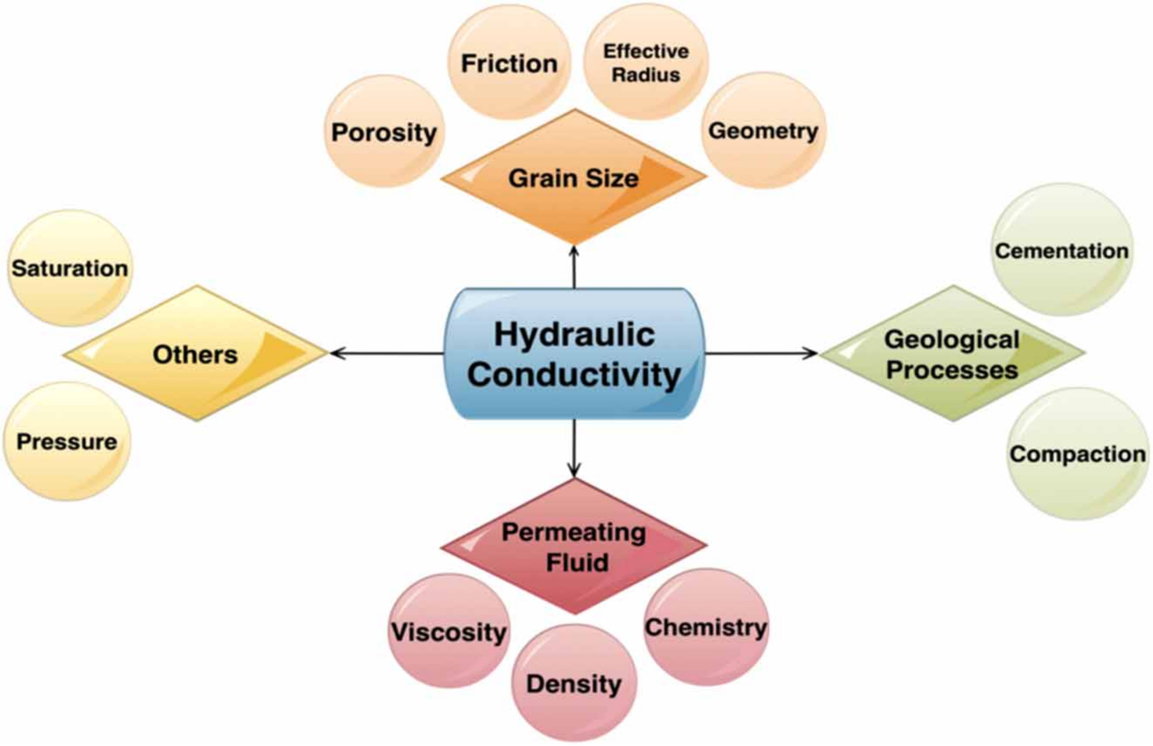
Hydraulic conductivity (k) is an important hydraulic parameter of porous media, and its accurate prediction plays a vital role in sub-surface flow investigations. The study uses the borehole soil samples to develop a k model using parameters, effective grain-size (d_{10}), and standard deviation (σ). The influence of d_{10} and σ on the k and evaluation of k values via four empirical models is also assessed in this study. For soil samples, the k increases with the increase in the d_{10} grain-size and decreases with the increase in the σ value. The evaluation of k via empirical models infers that the Hazen model performs well in the estimation of k values. The evaluation of k using various statistical indicators points towards low error statistics (MAE, RMSE, and BIAS) and high determination coefficient (R^2) between the measured and developed model-based k values, which substantiate the efficacy of the developed model as compared to the existing empirical models for estimating the k. To establish the versatility of the developed grain-size model, its validation was done using independent soil samples for estimating k values.

Key words: aquifer, groundwater, hydraulic conductivity, porous media

HIGHLIGHTS

- The research proposes a grain-size model for estimating the hydraulic conductivity of porous media by examining the effect of the σ/d_{10} parameter on k.
- The established hydraulic conductivity model served as a valuable tool for calculating aquifer yield and groundwater recharge with precise accuracy.

GRAPHICAL ABSTRACT



INTRODUCTION

The hydraulic conductivity (k) of porous media and its accurate assessment is important for a hydrogeologist in aquifer and groundwater studies (Leroueil *et al.* 2002). Initially, Henry Darcy explained the concept of hydraulic conductivity and defined it as the ease with which the flow of fluid takes place through the interconnected pore space (Pucko & Verbovsek 2015; Chandel *et al.* 2022a). For porous media, the studies concerning the k estimation are significant to govern the percolation ability of the permeable bed and soil sediments, as these factors are reliant on groundwater recharge (Chandel *et al.* 2022b).

In the previous studies, various researchers namely Parvazinia *et al.* (2006), Kundu *et al.* (2016), and Singh *et al.* (2021) studied different approaches for modelling the k of flow through porous media. The outcomes of these studies infer some restrictions, i.e., simulating the infinite extent of sub-surface flow. One of the important considerations is to control other factors that influence the k of porous media while examining the influence of individual parameters, i.e., standard deviation and mean and effective size (Lu *et al.* 2012). Pliakas & Petalas (2011) developed a statistical regression model by examining the correlation between the k and grain-size parameters and postulated that the developed model performed better in the estimation of k values. Salarashayeri & Siosemarde (2012) proposed a hydraulic conductivity equation using grain diameters, i.e., d_{10}, d_{50}, and d_{60}. The study recommended that the grain diameter (d_{10}) is an influencing factor for the k estimation of porous media. The M5 model tree regression approach was used to develop a k model based on the grain-size data (Naeej *et al.* 2017). Wang *et al.* (2017) proposed a k model by performing the dimensional analysis between the particle size parameters with the k. The developed equation performs better in the estimation of k values as compared to the existing empirical models. Ren & Santamarina (2018) estimated the k of porous media using the sediment and index characteristics i.e, void ratio, grain-size distribution, and surface area. Toumpanou *et al.* (2021) evaluated the k of the crushed sand-sized limestone using the pre-existing six empirical equations. Mujtaba *et al.* (2021) correlated the hydraulic conductivity with the different grain-sizes of sandy soil and concluded that the d_{10} grain-size shows better goodness of fit with the k as compared to the other grain-sizes. Khaja *et al.* (2022) developed an equation for the estimation of k of sandy aquifers using the grain-size data. The developed equation gives better results when the grain-size, i.e., d_{30} is considered to be an effective parameter.

From the existing literature, it has been seen that limited research work has been done to examine the influence of d_{10} and σ on the k of porous media. The standard deviation signifies the non-uniformity of the soil particles, whereas the effective grain-size represents the behavior of the entire grain-size pattern. The study incorporates two parameters, i.e., effective grain-size (d_{10}) and standard deviation (σ) for the development of a grain-size model. The present study is aimed:

(1) To investigate the influence of d_{10} and σ on the k value of porous media.
(2) To develop a grain-size model using parameters, i.e., σ & d_{10} and evaluate its efficacy in estimating the k of porous media.
(3) To validate the grain-size model using data set of independent soil samples.

MATERIALS AND METHODOLOGY

Materials

The study uses 27 borehole soil samples, which were attained during the ongoing drilling process from the Chamba district of Himachal Pradesh in India. Thin-walled sampler tubes were used to collect the undisturbed soil samples. For experimental work, the soil samples were collected at an interval of 3.5 m from the core material.

Methodology

The collected soil samples were subjected to the grain-size analysis to compute the mean and effective size. The pycnometer method was used to determine the specific gravity of soil samples, which is helpful in the determination of porosity. The grain-size curve (Figure 2) is used to determine the effective grain-size (d_{10}), whereas the standard deviation (σ) is determined (Rushton 2004) using the equation:

$$\sigma = \left(\sum (d_{50} - d_i)^2 * \Delta Z_i\right)^{\frac{1}{2}} \tag{1}$$

where, d_{50} – mean grain-size, ΔZ_i – total particles fraction, and d_i – particle size retained on a particular sieve.

Initially, the influence of d_{10} and σ on the k of soil samples were examined individually, and then by investigating the behaviour of k with the different σ/d_{10} values, a grain-size model has been proposed to predict hydraulic conductivity. For hydraulic conductivity estimation of soil samples, a constant head permeameter test has been performed. Permeameters of different diameters (5.08, 10.16, and 15.26 cm) have been used for k estimation as shown in Figure 1.

Figure 1 indicates the hydraulic conductivity measuring setup, which includes galvanized iron permeameters of different diameters. For each permeameter, the total and test lengths are 1 m and 0.46 m respectively. An overhead tank is provided above the permeameter outlet, which provides a continuous flow of water to the permeameter. The arrangement of pressure taping points is provided along the permeameter periphery, which helps in measuring the readings of the manometer. The volume of the water is measured using a measuring cylinder for a particular time interval. The standard methodology as described by Chandel & Shankar (2021) has been followed to determine the k of soil samples. During the k measurement, the temperature of the water is recorded at the start and end of the analysis using a digital thermometer (ASTM 2006).

Empirical models for k assessment

Based on the literature review, various empirical models that are used to evaluate the k of porous media have been used in this study. These empirical models relate the k with the grain-size, viscosity of fluid, porosity, sorting coefficient, and uniformity coefficient. Table 1 shows the empirical models with their boundary conditions used in the present study to evaluate the k values. In the empirical models, the ν and g values were taken as 0.885 mm^2/s and 981 cm/s^2 respectively.

Statistical performance indicators

In this study, several statistical indicators namely scatter index (S_i), BIAS, agreement index (I_a), determination coefficient (R^2), root mean square error (RMSE), and mean absolute error (MAE) have been used for quantitative

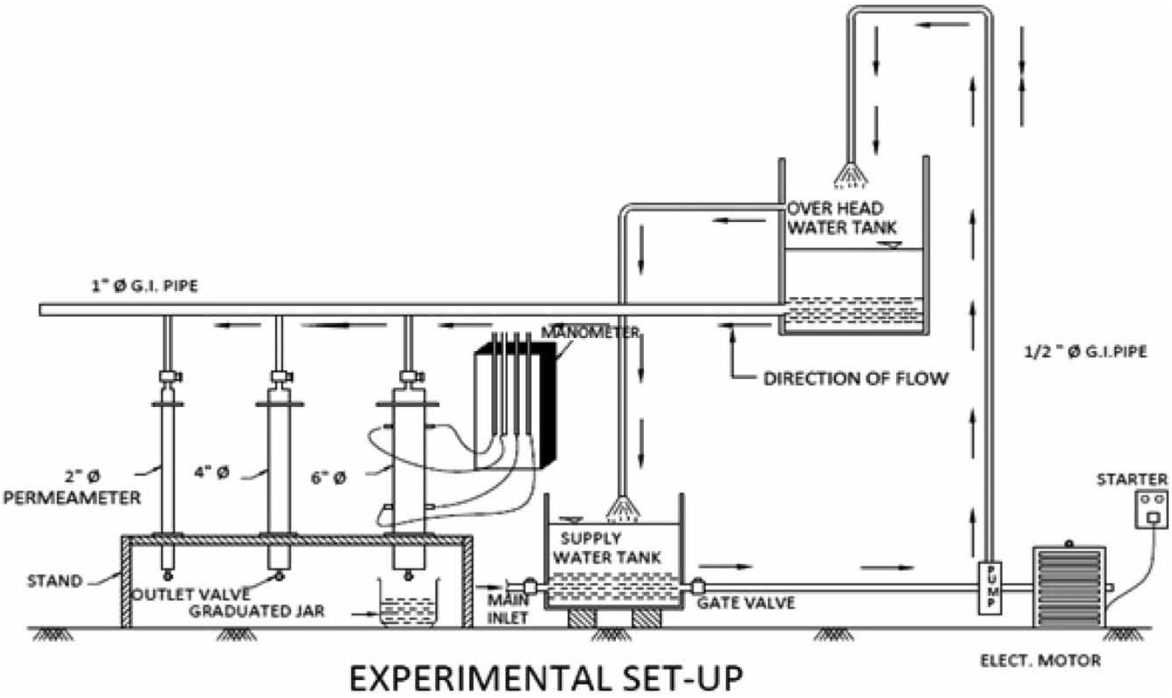


Figure 1 | Hydraulic conductivity measuring setup.

Table 1 | Empirical models for k assessment

Investigator	**Equation**	**Boundary conditions**
Hazen (1892)	$k = \frac{g}{v} * 6 \times 10^{-4} * [1 + 10\,(n - 0.26)] * d_{10}^{2}$	d_{10} (0.1–3 mm) $U < 5$
Kozeny (1927), Carman (1937, 1956)	$k = \frac{g}{v} * 8.3 \times 10^{-3} * \left[\frac{n^3}{(1-n)^2}\right] * d_{10}^{2}$	$d_{10} < 3.0$ mm
Chapuis *et al.* (2005)	$k = 1.412 * \frac{n^{2.35}}{(1-n)^{1.565}} * d_{10}^{1.565}$	d_{10} (0.03–3 mm)
Naeej *et al.* (2017)	$k = \frac{g}{\vartheta} * 1.84 \times 10^{-4} * d_{10}^{0.83} * U^{-0.55}$	suitable for sand $d_{10} < 3.0$ mm

where, U, uniformity coefficient i.e., d_{60}/d_{10}, and n, porosity.

evaluation. The statistical indicators (Chandel *et al.* 2021) are defined as:

$$BIAS = \sum_{i=1}^{Z} \frac{1}{Z} (C_i - M_i) \tag{2}$$

$$S_i = \frac{\sqrt{\frac{1}{Z} \sum_{i=1}^{Z} (C_i - M_i)^2}}{\bar{M}_i} \tag{3}$$

$$R^2 = \left[\frac{\sum_{i=1}^{Z} (M_i - \bar{M})(C_i - \bar{C})}{\sqrt{\sum_{i=1}^{Z} (M_i - \bar{M})^2 \sum_{i=1}^{Z} (C_i - \bar{C})^2}} \right]^2 \tag{4}$$

$$I_a = 1 - \frac{\sum_{i=1}^{Z} (C_i - M_i)^2}{\sum_{i=1}^{Z} |C_i - \bar{M}| + |M_i - \bar{M}|} \tag{5}$$

$$MAE = \frac{1}{Z}\sum_{i=1}^{Z} |M_i - C_i| \tag{6}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{Z} (M_i - C_i)^2}{Z}} \tag{7}$$

where, C_i and M_i represent the computed and measured k values respectively, and Z is the number of datasets. $\bar{C}$ and $\bar{M}$ denote the average values of computed and measured parameters, respectively.

RESULTS AND DISCUSSION

The hydraulic test and gradation analysis have been conducted on the 27 borehole soil samples. The data points of 15 soil samples were used to develop a k model by examining the influence of σ/d_{10} parameter on the k. The data set of remaining independent soil samples was used for the validation of the developed model.

Grain-size analysis

The grain-size analysis was performed to plot the grain-size curve between the particle size and percent finer. Figure 2 represents the grain-size curve for 15 soil samples. The grain sizes corresponding to the 10%, 30%, and 60% finer by weight i.e., d_{10}, d_{30}, and d_{60}, standard deviation, and uniformity coefficient values were determined using the grain-size curve. Whereas, the grain-size parameters (d_{10} and σ) for the remaining soil samples have been determined and provided in the validation section.

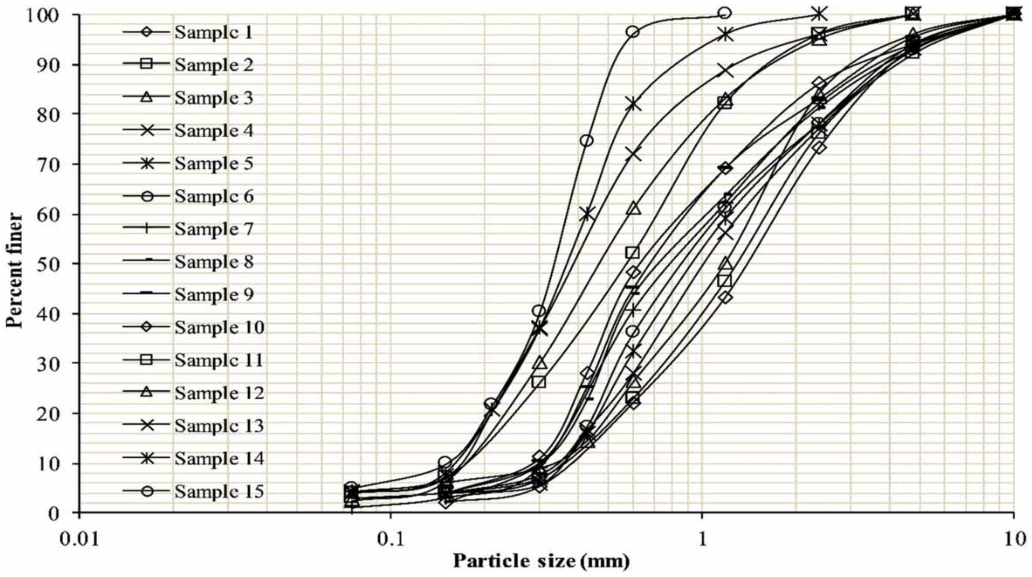


Figure 2 | Grain-size curve of 15 soil samples.

Table 2 represents the basic characteristics of the 15 soil samples. The σ and d_{10} values vary between 1.470 to 7.100 and 0.173 to 0.386 mm respectively.

Variation of hydraulic conductivity with d_{10} and σ

Figure 3(a) represents a linear variation of k values, which are obtained from the three permeameters with the different values of effective grain-size (d_{10}). The increase in the d_{10} grain-size provides more interconnected

Table 2 | Basic characteristics of the soil samples

Sample no.	d_{10} (mm)	d_{30} (mm)	d_{50} (mm)	d_{60} (mm)	n^a	U^a	σ^a
1	0.386	0.821	1.450	1.850	0.359	4.793	1.470
2	0.373	0.774	1.330	1.720	0.363	4.611	1.560
3	0.358	0.690	1.180	1.530	0.370	4.274	1.640
4	0.347	0.631	1.050	1.400	0.375	4.035	1.790
5	0.342	0.575	0.980	1.240	0.385	3.626	1.980
6	0.330	0.544	0.920	1.160	0.387	3.515	2.190
7	0.325	0.499	0.850	1.120	0.389	3.446	2.460
8	0.301	0.486	0.785	1.070	0.386	3.555	2.780
9	0.297	0.468	0.720	0.962	0.394	3.239	2.980
10	0.278	0.442	0.650	0.929	0.392	3.342	3.320
11	0.225	0.346	0.570	0.754	0.392	3.351	3.780
12	0.191	0.300	0.490	0.590	0.398	3.089	4.130
13	0.187	0.264	0.410	0.497	0.410	2.658	4.890
14	0.178	0.260	0.370	0.425	0.418	2.388	5.870
15	0.173	0.252	0.335	0.372	0.426	2.150	7.100

[a] represents the unitless parameters.

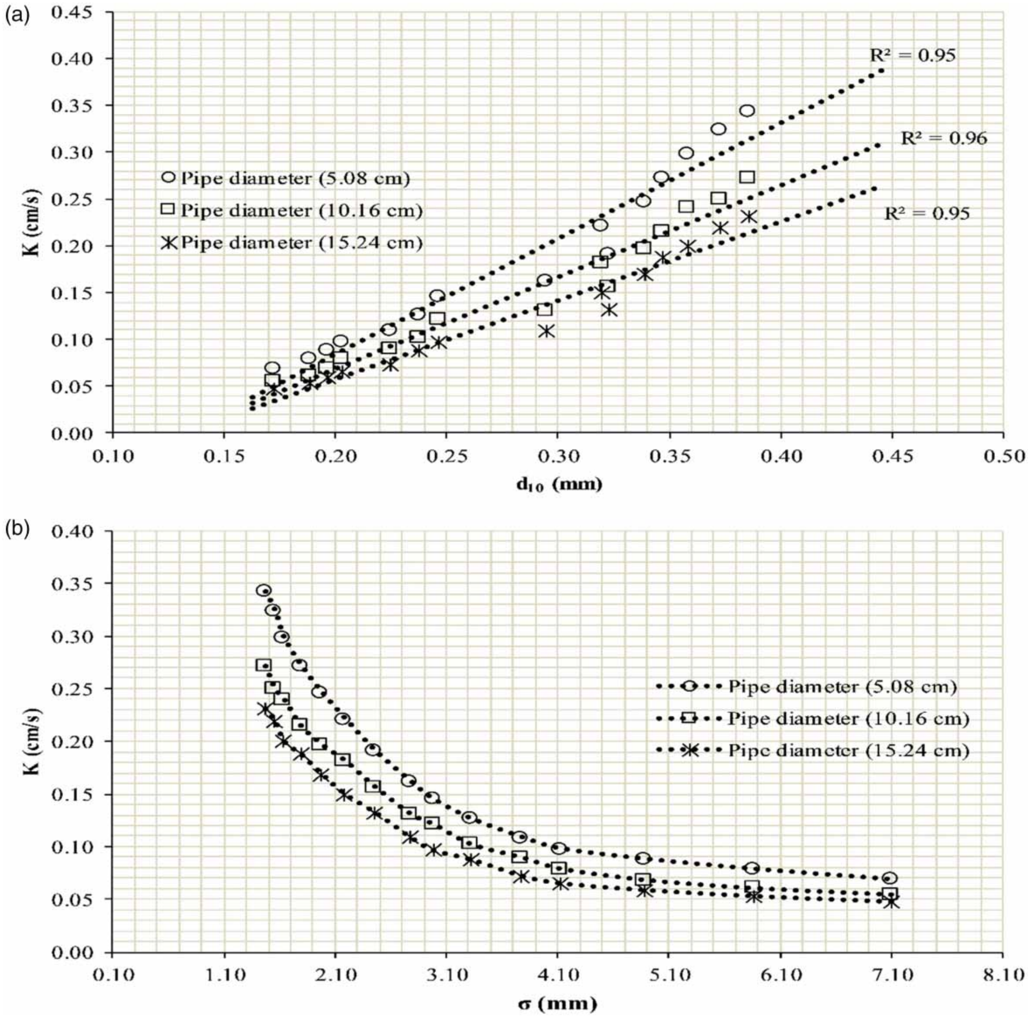


Figure 3 | Hydraulic conductivity variation with (a) d_{10} (b) σ.

space between the voids for the fluid flow, which results in an increase in the k value. The outcome of the study is in close agreement with the findings of Cabalar & Akbulut (2016).

Figure 3(b) indicates that the hydraulic conductivity decreases with the increase in the σ values, which vary from 1.47 to 7.10. The σ value more than unity signifies the non-uniformity of soil particles. In this study, the non-uniformity of soil particles increases with the increase in the σ value which results in providing more compactness to the porous particles and thus results in the decreased k value.

Variation of k with σ/d_{10}

The hydraulic conductivity variation was examined by plotting the k with different σ/d_{10} values for different diameter permeameters.

The σ/d_{10} parameter effectively incorporates the influence of non-uniformity and gradation characteristics on the k of porous media. Figure 4 shows that the k decreases with the increase in the σ/d_{10} value. The curve is concave upward and meets the lower limiting value asymptotically. In Figure 4, the trend of the curve implies that the result of the study is in line with the outcomes of Pliakas & Petalas (2011).

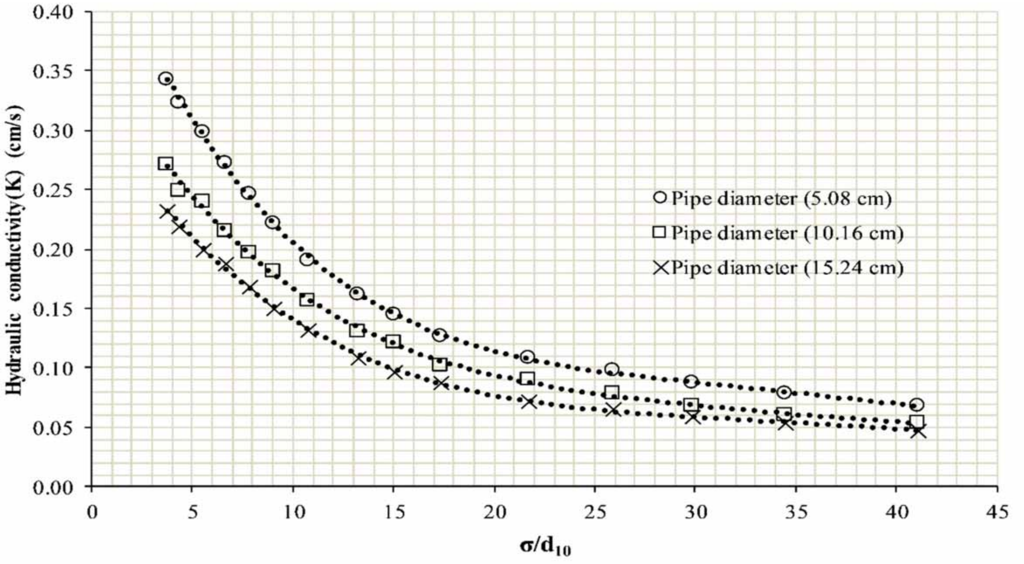


Figure 4 | Variations of k with σ/d_{10}.

Grain-size model development

The data points of 15 soil samples have been used for the development of a grain-size model. For model development, the grain-size parameters (σ and d_{10}) have been integrated to form a dimensionless parameter 'σ/d_{10}'. The equation of the developed model is derived by investigating the variations of the σ/d_{10} parameter with the hydraulic conductivity values obtained from the three different diameter permeameters for 15 soil samples i.e., a total number of 45 k versus σ/d_{10} variations were examined for model development. The 'σ/d_{10}' parameter in the developed model includes coefficients of degree 0–4. For the development of the model, the principle of least-squares approach is used in this study (Wang *et al.* 2017).

The developed hydraulic conductivity model is:

$$k = \beta * \left[a_0 + \left\{ \int_{i=1}^{i=4} a_i * \left(\frac{\sigma}{d_{10}} \right)^i \right\} \right] \qquad \left(3.805 \leq \frac{\sigma}{d_{10}} \leq 41.066 \right) \tag{8}$$

where, β is a parameter that considers the soil particle's compactness, particle roughness, and porous media extent. The β values for different permeameter diameters are:

Permeameter diameter (cm)	**β values**
5.08	1.23
10.16	0.96
15.24	0.82

The observed β suggests that its β value is smaller for maximum and larger for minimum, permeameter size. The outcome of the study infers that the increase in the porous media extent results in an insignificant β value (Zieba 2017).

The values of empirical constants i.e., a_0, a_1, a_2, z_3, & a_4 are:

$a_0 = 0.388$, $a_1 = 0.0327$, $a_2 = 0.0013$, $a_3 = 2.56 \times 10^{-5}$, & $a_4 = 2 \times 10^{-7}$

For the k estimation, the developed model is:

$$k = \lambda * \left[2 \times 10^{-7}\left(\frac{\sigma}{d_{10}}\right)^4 - 2.56 \times 10^{-5}\left(\frac{\sigma}{d_{10}}\right)^3 + 0.0013\left(\frac{\sigma}{d_{10}}\right)^2 - 0.0327\left(\frac{\sigma}{d_{10}}\right) + 0.388\right] \tag{9}$$

Table 3 represents the developed model-based and experimentally measured k values for 15 soil samples.

Table 3 | Developed model-based and measured k values

		($k_{measured}$) Permeameter diameter (cm)			(k_{model}) Permeameter diameter (cm)		
Sample no.	**σ/d_{10}**	**5.08**	**10.16**	**15.24**	**5.08**	**10.16**	**15.24**
1	3.805	0.342	0.271	0.232	0.346	0.270	0.231
2	4.390	0.323	0.249	0.219	0.330	0.257	0.220
3	5.539	0.298	0.240	0.200	0.300	0.234	0.200
4	6.669	0.272	0.215	0.188	0.273	0.213	0.182
5	7.876	0.246	0.197	0.169	0.248	0.194	0.165
6	9.058	0.221	0.181	0.150	0.226	0.176	0.151
7	10.787	0.190	0.156	0.132	0.199	0.155	0.132
8	13.255	0.162	0.131	0.109	0.168	0.131	0.112
9	15.104	0.145	0.121	0.097	0.150	0.117	0.100
10	17.376	0.126	0.102	0.088	0.133	0.104	0.089
11	21.754	0.109	0.090	0.072	0.114	0.089	0.076
12	25.964	0.098	0.079	0.065	0.106	0.083	0.071
13	29.868	0.088	0.068	0.059	0.104	0.082	0.070
14	34.467	0.078	0.061	0.053	0.093	0.076	0.064
15	41.066	0.069	0.054	0.048	0.082	0.065	0.052

Further, the experimentally measured k values have been compared with the developed model-based k values. Figure 5 indicates a relatively good agreement between the measured and developed model-based k values.

Further, the uncertainty analysis of the developed model, i.e., Equation (9) has been performed (Parsaie & Haghiabi 2021). In Equation (9), the dependent parameter is k, whereas the independent parameters are σ & d_{10}. Initially, for uncertainty analysis, the σ value remains constant, while the d_{10} value increases from the baseline value up to 20%, resulting in an increase in the k value by 5.5%. The k value decreases up to 6.2%, when the σ value increases from 0 to 20%, while the d_{10} value remains constant. Based on the results, both the σ and d_{10} parameters are dependent on k, while the d_{10} is positively sensitive to k and σ is inversely sensitive to k.

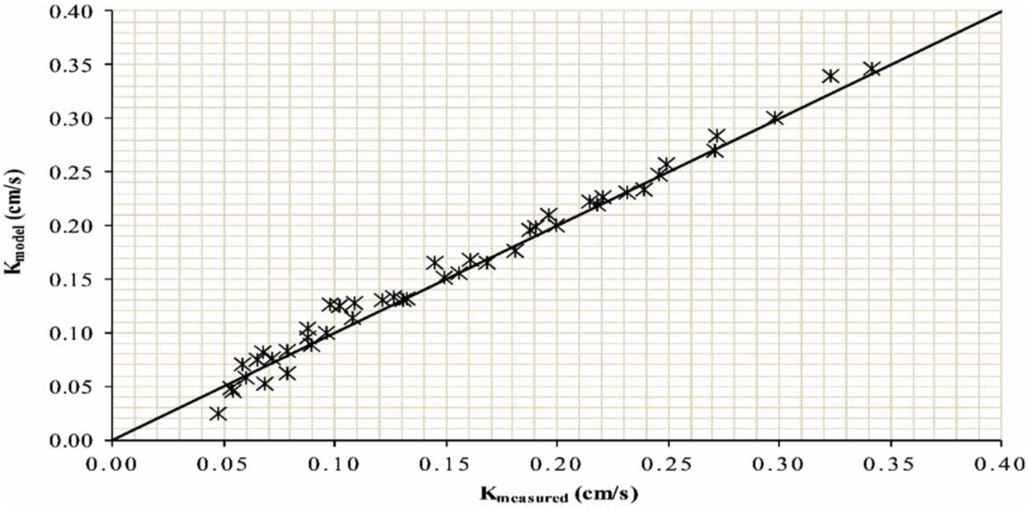


Figure 5 | Measured and model-based comparison of k.

k evaluation using empirical models

In this study, four empirical models have been used to evaluate the k values. Table 2 represents the grain-size parameters that were used to calculate the k values via empirical models.

From Figure 6, it has been observed that for soil samples, the Hazen model provides the closest fit to the measured k values, followed by the Kozeny-Carman model. Because it takes into account the grain-size curve, porosity, and effective grain-size, the Hazen model calculates k more precisely than the other models (Ishaku *et al.* 2011; Chandel & Shankar 2022). Also, as evident in Figure 6, the developed model exhibits reasonably good agreement with the measured K values when compared to the empirical models investigated in the study.

Further, various statistical indicators were used to evaluate the quantitative assessment of the developed model for different diameter permeameters as given in Table 4.

The BIAS, MAE, S_i, and RMSE values vary from 0 to ∞ and R^2 and I_a from 0 to 1 (Rosas *et al.* 2014). Lower values of MAE, S_i, BIAS, and RMSE, and values closer to 1 for I_a and R^2 point to a better agreement between the observed and measured parameters (Naeej *et al.* 2017). The BIAS, S_i, MAE, RMSE, R^2, and I_a values for the developed model are 0.006, 0.039, 0.005, 0.009, 0.978, and 0.976 for 5.08 cm, 0.003, 0.051, 0.008, 0.005, 0.984, and 0.974 for 10.16 cm, and 0.004, 0.041, 0.007, 0.006, 0.962, and 0.981 for 15.24 cm diameter permeameters respectively. The values of statistical indicators for the developed model establish its efficacy in estimating the k of porous media.

Validation of the grain-size model

The grain-size parameters (d_{10} and σ) of the remaining 12 soil samples have been determined and used for validation. For computing the k value, the developed model includes a parameter, i.e., σ/d_{10}. Therefore, for these 12 soil samples, the σ/d_{10} values have been determined as shown in Table 5.

For validation, the hydraulic conductivity for the 12 soil samples has been computed via the grain-size model and then compared with the permeameter-based measured values as shown in Figure 7.

Figure 7 indicates a fairly good agreement between the measured and developed model-based predicted k values. For the developed model the BIAS, I_a, R^2, S_i, RMSE, and MAE values during validation are 0.038, 0.885, 0.934, 0.048, 0.016, and 0.028 respectively, which substantiate the performance of the grain-size model in estimating the hydraulic conductivity of porous media.

CONCLUSIONS

The present study is focused on developing a hydraulic conductivity model using grain-size parameters i.e., d_{10} and σ. The grain-size model comprises a factor 'β' which inherits the particle roughness, porous media extent,

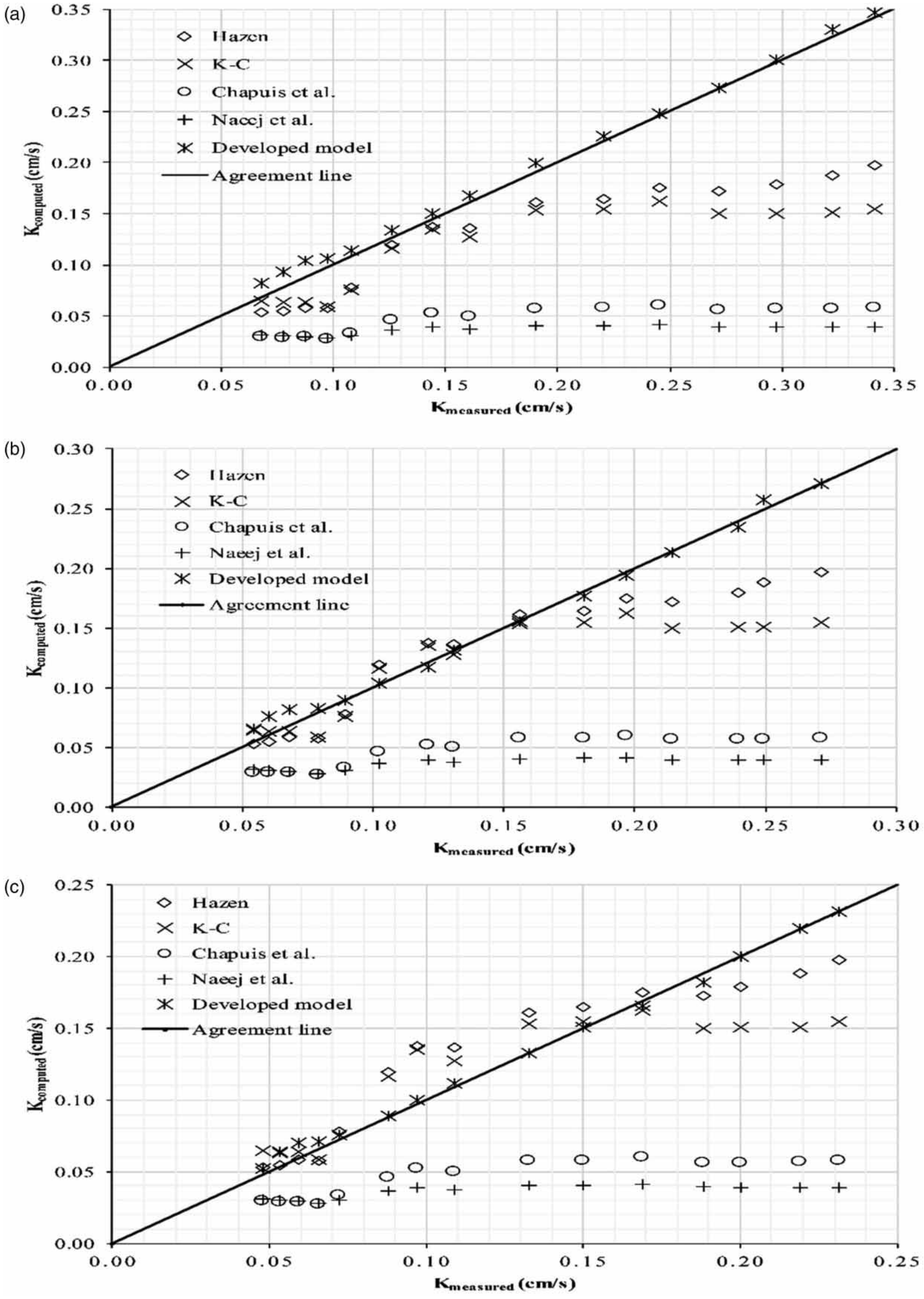


Figure 6 | Evaluation of k values for (a) 5.08, (b) 10.16, & (c) 15.24 cm permeameters size.

and compactness of porous media. The increase in the porous media extent results in an insignificant β value. For borehole soil samples, the influence of d_{10} and σ on the hydraulic conductivity elucidate that the k increases with the increase in the d_{10} grain-size and decreases with the increase in the σ value. The evaluation of k values via empirical models infers that the Hazen model performs well in k estimation, followed by the Kozeny-Carman

Table 4 | Grain-size model quantitative assessment via statistical indicators

	Statistical indicators					
Permeameter Diameter (cm)	**BIAS**	**S_i**	**R^2**	**I_a**	**MAE**	**RMSE**
5.08	0.006	0.039	0.978	0.976	0.005	0.009
10.16	0.003	0.051	0.984	0.974	0.008	0.005
15.24	0.004	0.041	0.962	0.981	0.007	0.006

Table 5 | Predicted k via the grain-size model

		($k_{predicted}$)			**($k_{measured}$)**		
		Permeameter diameter (cm)			**Permeameter diameter (cm)**		
Sample no.	**σ/d_{10}**	**5.08**	**10.16**	**15.24**	**5.08**	**10.16**	**15.24**
1	3.519	0.355	0.277	0.236	0.364	0.268	0.227
2	3.831	0.345	0.270	0.230	0.325	0.255	0.222
3	4.800	0.319	0.249	0.212	0.314	0.244	0.208
4	5.714	0.295	0.231	0.197	0.275	0.204	0.227
5	4.930	0.315	0.246	0.210	0.321	0.252	0.202
6	4.215	0.335	0.261	0.223	0.312	0.228	0.260
7	5.818	0.293	0.229	0.195	0.248	0.185	0.168
8	6.920	0.268	0.209	0.178	0.275	0.215	0.180
9	7.982	0.246	0.192	0.164	0.205	0.168	0.138
10	10.792	0.199	0.155	0.132	0.158	0.145	0.109
11	15.850	0.144	0.112	0.096	0.118	0.082	0.069
12	20.160	0.119	0.093	0.080	0.091	0.078	0.056

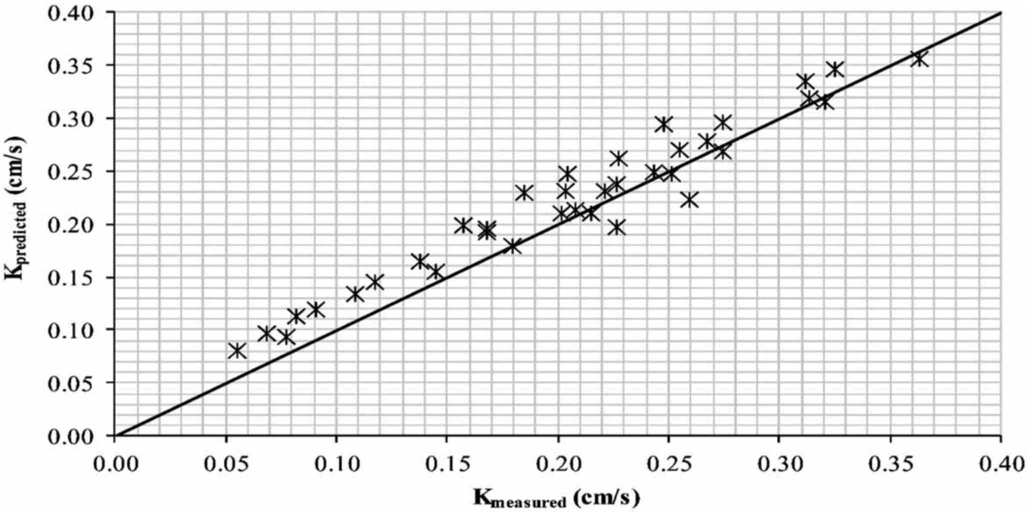


Figure 7 | Comparison between measured and predicted k.

model. The quantitative assessment of the grain-size model via the statistical indicators substantiates its efficacy in estimating the k. Also, using the independent data set, the study validates the performance of the grain-size model in estimating k. The study recommends further investigations to examine the influence of particle and wall roughness on the k of porous media.

DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

CONFLICT OF INTEREST

The authors declare there is no conflict.

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