Study on Application of Three Methods for Calculating the Dispersion Parameters – A Case Study in Yinchuan, China

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Abstract: ***In this paper, linear graphical method, moment method and inverse function method are first applied in the laboratory test of one dimensional sand column device, determining the longitudinal dispersion coefficient. The longitudinal dispersions for five groups of sand taken from 20cm below the ground surface in the Oil Refinery of China Petroleum Ningxia Filial are obtained. On this basis, the problems within the calculation process when the three kinds of methods are applied into actual data were discussed. It can be readily concluded that the three values of dispersion coefficients are approximate, and the errors caused by the subjective factors of artificial mapping and numerical reading were avoided. The inverse function method is recommended to apply for the high accuracy, sample calculation process, less known conditions and better linearity.***

Keywords: longitudinal dispersion coefficient; laboratory test; linear graphical method; moment method; inverse function method.

1. Introduction

Dispersion parameter is the foundation of researching the groundwater pollutant regular pattern and predicting the water quality (Liu et al. 2011). The convection dispersion and molecular diffusion in the porous medium are named as hydrodynamic dispersion coefficient. It is a comprehensive reflection coefficient of solute, soil, and it is not only related to the condition of porous medium and the properties of solute, but also depended on the effect of moisture content and the velocity of pore water (Song et al. 1998). The dispersion parameter is indispensable for the study of migration law of chemical fertilizers, pesticides and heavy metals in farmland, the monitoring of water movement and salt in saline and alkaline land, and the protection of the groundwater resource. The macroscopic parameters that quantify the solute dispersion in porous medium are longitudinal and transverse dispersion coefficients (Aggelopoulos et al. 2007). There are many researches about hydrodynamic dispersion in the world. Several methods based on analytical solutions have been developed particularly in order to determine the hydrodispersive characteristics from the tracer experiments (Wang et al. 1987; Fried 1975; Sauty 1978). The theory of hydrodynamic dispersion in porous materials has been developed on a series of boundary conditions (Bachmat and Bear 1964; Fried 1975; Hibsch and Kreft 1979; Harleman and Rumer 1963). Delgado (2007) has studied the longitudinal and transverse dispersion in porous media. A series of laboratory tests were carried out on artificially produced particle mixtures (Klotz 1980; Klotz and Moser 1974). For the measurement of the dispersion parameter in saturated aquifer, the commonly used and mature method is laboratory dispersion test with the column devices. At present, the laboratory dispersion test is mostly used in this situation: the steady flow, continuous tracer injection of definite concentration at one side of the column. Get the change of concentration of different time at each section of one dimensional sand column, repeatedly (Li et al. 1983). For the calculation of dispersion coefficient, the most widely used method is the method of breakthrough curves (Zhang et al. 2003). In addition, Guo J Q also put forward a series of solutions aiming at one dimensional dispersion of groundwater. Such as linear graphical method (Guo et al. 1997), the moment method (Guo et al. 1997) and inverse function method (Guo et al. 1999). These methods have not been used in practice science they were put forward. Here, five groups of actual data are calculated by the three methods.

2. Methods

The tracer of concentration c0 is continuously and steadily poured into the top of the semi-infinite columnar aquifer. Seepage is uniform flow. One-dimensional dispersion, and there isn't other source sink term. The mathematical model (1) for this problem is listed as follows:

$$\begin{cases} -\dfrac{\partial c}{\partial t} = D_L \dfrac{\partial^2 c}{\partial x^2} - V\dfrac{\partial c}{\partial x} & 0 < x < \infty, t > 0 \\ c(x,0) = 0 & 0 < x < \infty \\ c(0,t) = c_0 & t > 0 \\ c(\infty,t) = 0 & t < 0 \end{cases} \qquad (1)$$

The solution of this mathematical model is:

$$c(x,t) = c_0 \exp(\frac{Vt}{2D_L}) L^{-1}[\frac{1}{p}\exp(-k\sqrt{b+p})] = \frac{c_0}{2}[erfc(\frac{x-Vt}{2\sqrt{D_L t}}) + \exp(\frac{V_x}{D_L})erfc(\frac{x+Vt}{2\sqrt{D_L}})] \qquad (2)$$

Or it can be written as:

$$\bar{c} = \frac{c(x,t)}{c_0} = \frac{1}{2}[erfc(\frac{x-Vt}{2\sqrt{D_L t}}) + \exp(\frac{V_x}{D_L})erfc(\frac{x+Vt}{2\sqrt{D_L}})] \qquad (3)$$

When x is sufficiently large, the second term is too small compared with the first term in equation (3). Then the second term can be neglected, and the equation (3) can be written as:

$$\frac{c(x,t)}{c_0} = \frac{1}{2} erfc(\frac{x-Vt}{2\sqrt{D_L t}}) \quad (4)$$

Where, c(x,t) - the tracer concentration at t time, x coordinate.

c0 – tracer concentration at the injection site.
x – vertical coordinate.
t – time coordinate.
V – seepage velocity.
DL – longitudinal dispersion coefficient.
erfc() – complementary error function, and its expression is as follows.

$$erfc(\frac{x-Vt}{2\sqrt{D_L t}}) = 1 - \frac{1}{2\pi}\int_{-\infty}^{\frac{x-Vt}{2\sqrt{D_L t}}} \exp(-\frac{\eta^2}{2}) d\eta \quad (5)$$

Based on the above two equations the following methods are put forward.

2.1 Linear graphical method

Linear graphical method is put forward by Guo J Q (1997). This solution cites the theory in literature (Wang et al. 1987) and is obtained via proper conversion conducted for approximate analytic solution during the dispersion test on the condition of one dimensional, stable state and injection of tracer with definite concentration at one side of semi-infinite sand column. Take the injection site as the origin of coordinates, and the groundwater flow direction as the direction of x axis. Based on equations (4), (5) and the integral principle of variable upper limit, the linear equation (6) can be obtained after taking the logarithm. The linear constant is a function of longitudinal dispersion coefficient, so it is feasible to determine dispersion coefficient with linear diagrammatic solution or by linear regression.

$$T = a + by \quad (6)$$

Where,

$$a = -\frac{1}{2}\ln(4\pi D_L) \quad (7)$$

$$b = -\frac{1}{4D_L} \quad (8)$$

The following formulas can be used for data transformation:

$$y_i = \frac{x - Vt_i}{\sqrt{t_i}} \quad (9)$$

$$T_{i+1/2} = \ln(-\frac{\overline{c_{i+1}} - \overline{c_i}}{y_{i+1} - y_i}) \quad (10)$$

$$y_{i+1/2} = -\frac{1}{4}(y_{i+1} + y_i) \quad (11)$$

Here linear diagrammatic solution or linear regression method can be used to solve the value of DL after confirming the value a, b with the following equations.

$$D_L = \frac{1}{4\pi}\exp(-2a) \quad (12)$$

Or

$$D_L = -\frac{1}{4b} \quad (13)$$

2.2 Moment method

The moment method (Guo et al. 1997) is derived with forepart inference result of linear graphical method. And its final form is the same as normal probability density function of variance $\delta^2 = 4D_L$, and mathematical expectation m=0. As follows:

$$f(y) = \frac{1}{\sqrt{4\pi D_L}} Exp(-\frac{y^2}{4D_L}) \quad (14)$$

In equation (14), the expression of y is the same as equation (9). The value of δ^2 can be worked out with the formula $\delta^2 = M_2/M_0$. Then the value of dispersion coefficient (D_L) can be calculated from the formula $D_L = \delta^2/4$. Some equations needed in the computational process are listed as follows:

$$\bar{c} = \frac{c(x,t)}{c_0} \quad (15)$$

$$f(y_{i+1/2}) = -\frac{\overline{c_{i+1}} - \overline{c_i}}{y_{i+1} - y_i} \quad (16)$$

$$M_2 = \sum_{i=1}^{n-1}(-\frac{c_{i+1} - c_i}{y_{i+1} - y_i}) \cdot \frac{(y_{i+1} + y_i)^2}{4} \cdot (y_{i+1} - y_i) \quad (17)$$

$$M_0 = \sum_{i=1}^{n-1}(-\frac{c_{i+1} - c_i}{y_{i+1} - y_i}) \cdot (y_{i+1} - y_i) \quad (18)$$

2.3 Inverse function method

The linearization idea is adopted within the process of the inverse function method's putting forward (Guo et al. 1999). When data is sufficient the equation (5) can be transformed into the following equation.

$$G_t = a + bt \quad (19)$$

Where,

$$G_t = t^{\frac{1}{2}} arcN(y) \quad (20)$$

The expression of y is the same as equation (9). ArcN(y) means the inverse function of the normal function. It can be got from pegging normal function table. The value of a and b may be obtained through linear diagrammatic solution or linear regression method by using the serial data G_t~t. In equation (19), the expressions of a and b can be written as followings:

$$a = \frac{x_0}{\sqrt{2D_L}} \quad (21)$$

$$b = -\frac{V}{\sqrt{2D_L}} \quad (22)$$

Once the value a and b are obtained, the value of dispersion coefficient (D_L) and seepage velocity (V) can be got with equation (21) and (22).

3. Study Area and Data Collection

3.1 Description of study area

The oil refinery of China Petroleum Ningxia filial is located in the south of Yinchuan City. The study area is located in the alluvial-proluvial plain, and the lithology of the phreatic aquifer mainly is fine sand. Here, the groundwater flows from southwest to northeast. Pollutants may migration with groundwater flow to south water source protection area. In this experiment, the sand column uses phreatic aquifer core of the drill hole in the oil refinery. The specification of testing apparatus depends on the sample size. The bigger size the sample, the larger the seepage pipe diameter required. And the seepage length must be more 3~4 times than pipe diameter (Zhang et al. 1993). Five groups of laboratory tests are arranged with one dimensional column device. The process of the tests is in accordance with the description in literature (Li et al. 2012).

3.2 Data collection

The five groups of data measured in laboratory dispersion test are called data1, data2, data3, data4 and data5. As shown in table1 to table5.

Table 1: Data 1

t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$
0.000	0.0006	0.125	0.0016	0.222	0.0000	0.319	0.7557	0.417	0.9685
0.021	0.0002	0.139	0.0001	0.236	0.0032	0.333	0.8069	0.431	1.0000
0.042	0.0009	0.153	0.0014	0.250	0.0259	0.347	0.8581	0.444	0.9764
0.063	0.0002	0.167	0.0008	0.264	0.1350	0.361	0.9054	0.458	0.9819
0.083	0.0005	0.181	0.0006	0.278	0.3360	0.375	0.9606		
0.097	0.0009	0.194	0.0005	0.292	0.4759	0.389	0.9567		
0.111	0.0006	0.208	0.0006	0.306	0.4995	0.403	0.9937		

Table 2: Data 2

t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$
0.000	0.0012	0.486	0.0032	0.819	0.0061	1.153	0.1342	1.563	0.7355
0.021	0.0012	0.500	0.0028	0.833	0.0084	1.167	0.1730	1.583	0.7520
0.042	0.0048	0.514	0.0018	0.847	0.0095	1.181	0.1914	1.604	0.7650
0.063	0.0034	0.528	0.0026	0.861	0.0114	1.194	0.1979	1.625	0.7846
0.083	0.0036	0.542	0.0043	0.875	0.0126	1.208	0.2144	1.646	0.7880
0.104	0.0044	0.556	0.0015	0.889	0.0130	1.222	0.2455	1.667	0.8145
0.125	0.0032	0.569	0.0022	0.903	0.0153	1.236	0.2766	1.688	0.8268
0.139	0.0058	0.583	0.0018	0.917	0.0168	1.250	0.3007	1.708	0.8483
0.153	0.0015	0.597	0.0038	0.931	0.0197	1.264	0.3157	1.729	0.8652
0.167	0.0045	0.611	0.0030	0.944	0.0233	1.278	0.3372	1.750	0.8805
0.181	0.0045	0.625	0.0043	0.958	0.0258	1.292	0.3671	1.771	0.8306
0.194	0.0025	0.639	0.0030	0.972	0.0305	1.306	0.3802	1.792	0.9074
0.222	0.0033	0.653	0.0030	0.986	0.0339	1.319	0.4009	1.813	0.9170
0.236	0.0020	0.667	0.0016	1.000	0.0360	1.333	0.4297	1.833	0.9308
0.250	0.0031	0.681	0.0026	1.014	0.0483	1.354	0.4527	1.854	0.9438
0.264	0.0036	0.694	0.0034	1.028	0.0523	1.375	0.4911	1.875	0.9599
0.278	0.0010	0.708	0.0030	1.042	0.0567	1.396	0.5160	1.896	0.9599
0.333	0.0028	0.722	0.0090	1.056	0.0655	1.417	0.5337	1.917	0.9745
0.361	0.0036	0.736	0.0051	1.069	0.0805	1.438	0.5820	1.938	0.9711
0.389	0.0023	0.750	0.0009	1.083	0.0840	1.458	0.5885	1.958	1.0029
0.417	0.0050	0.764	0.0045	1.097	0.1031	1.479	0.6196	1.979	0.9876
0.444	0.0054	0.778	0.0054	1.111	0.1154	1.500	0.6944	2.000	0.9972
0.458	0.0046	0.792	0.0053	1.125	0.1242	1.521	0.6952	2.021	1.0060
0.472	0.0034	0.806	0.0053	1.139	0.1308	1.542	0.7136	2.042	1.0064

Table 3: Data 3

t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$
0.000	0.0009	0.208	0.0014	0.375	0.1960	0.542	0.8880	0.708	0.9787
0.021	0.0014	0.222	0.0021	0.389	0.3061	0.556	0.9025	0.722	0.9787
0.042	0.0006	0.236	0.0021	0.403	0.4348	0.569	0.9025	0.736	0.9787
0.063	0.0008	0.250	0.0014	0.417	0.5483	0.583	0.9094	0.750	0.9977
0.083	0.0008	0.264	0.0023	0.431	0.6587	0.597	0.9254	0.764	0.9939
0.104	0.0012	0.278	0.0037	0.444	0.6907	0.611	0.9444	0.778	0.9962
0.125	0.0008	0.292	0.0048	0.458	0.7380	0.625	0.9482	0.792	0.9756
0.139	0.0000	0.306	0.0052	0.472	0.7882	0.639	0.9474	0.806	1.0000
0.153	0.0013	0.319	0.0086	0.486	0.8172	0.653	0.9634		
0.167	0.0018	0.333	0.0216	0.500	0.8339	0.667	0.9650		
0.181	0.0020	0.347	0.0624	0.514	0.8454	0.681	0.9254		
0.194	0.0002	0.361	0.1118	0.528	0.8911	0.694	0.9634		

Table 4: Data 4

t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$
0.000	0.0007	0.194	0.0000	0.347	0.4564	0.500	0.9423	0.653	0.9708
0.021	0.0015	0.208	0.0011	0.361	0.5425	0.514	0.9468	0.667	0.9656
0.042	0.0010	0.222	0.0019	0.375	0.6294	0.528	0.9393	0.681	0.9356
0.063	0.0007	0.236	0.0022	0.389	0.7147	0.542	0.9558	0.694	0.9768
0.083	0.0001	0.250	0.0071	0.403	0.7784	0.556	0.9633	0.708	0.9880
0.104	0.0001	0.264	0.0210	0.417	0.8420	0.569	0.9558	0.722	1.0000
0.125	0.0013	0.278	0.0552	0.431	0.8405	0.583	0.9925	0.736	0.9850
0.139	0.0004	0.292	0.1176	0.444	0.9244	0.597	0.9468	0.750	0.9910
0.153	0.0004	0.306	0.1801	0.458	0.9094	0.611	0.9468	0.764	0.9948
0.167	0.0005	0.319	0.2726	0.472	0.9319	0.625	0.9730		
0.181	0.0019	0.333	0.3493	0.486	0.9356	0.639	0.9708		

Table 5: Data 5

t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$	t(d)	$\bar{C}$
0.000	0.0008	0.181	0.0007	0.319	0.7962	0.458	0.9743	0.597	0.9638
0.021	0.0000	0.194	0.0006	0.333	0.8317	0.472	0.9758	0.611	0.9887
0.042	0.0008	0.208	0.0023	0.347	0.8506	0.486	0.9774	0.625	0.9796
0.063	0.0010	0.222	0.0128	0.361	0.8815	0.500	0.9660	0.639	0.9774
0.083	0.0006	0.236	0.0675	0.375	0.8898	0.514	0.9683	0.708	1.0000
0.104	0.0004	0.250	0.2004	0.389	0.8958	0.528	0.9698	0.722	0.9985
0.125	0.0013	0.264	0.3502	0.403	0.9245	0.542	0.9826	0.736	1.0000
0.139	0.0011	0.278	0.4906	0.417	0.9457	0.556	0.9547		
0.153	0.0015	0.292	0.6536	0.431	0.9547	0.569	0.9532		
0.167	0.0011	0.306	0.7358	0.444	0.9638	0.583	0.9623		

4. Results and discussion

Table 6 shows the results of dispersion coefficient with three methods and five groups of data. The average value of dispersion coefficient (DL) with linear graphical method, moment method and inverse function method is respectively 0.068 m^2/d, 0.056 m^2/d and 0.081 m^2/d. It can be easily found that the three values are approximate. In inverse function method, the value of seepage velocity (V) calculated is very approximate to that measured, which brings convenience to the column experiment.

Table 6: Calculation results with the three methods

Data		Data1	Data2	Data3	Data4	Data5	Average value
x(m)		1.3	1.29	1.3	1.3	1.29	
V(m/d)		4.6656	0.948	3.3336	3.8976	5.0064	
Linear graphical method	a	-0.2676	0.4628	-0.029	-0.277	-0.2331	
	b	-2.8921	-11.5515	-6.5338	-2.8137	-2.3529	
	D_L(m^2/d)	0.0864	0.0216	0.0383	0.0889	0.1063	0.068
Moment method	M_2	-0.1287	-0.2	-0.1595	-0.1942	-0.4358	
	M_0	-0.9816	-1.0051	-0.9986	-0.9933	-1	
	D_L(m^2/d)	0.0328	0.0497	0.0399	0.0489	0.1089	0.056
Inverse function method	a	4.398	5.729	3.152	2.796	2.398	
	b	-14.37	-4.155	-7.079	-7.751	-8.235	
	D_L(m^2/d)	0.0437	0.0254	0.0851	0.1081	0.1447	0.081
	V(m/d)	4.2476	0.9356	2.9196	3.6038	4.43	

On the condition of DL = 0.5 m^2/d, c0 = 333.33 g/m3, V = 5 m^2/d, x = 1 m, the data c/c0 ~ ti can determined with equation (5), listed in table 7 (Guo 1997, 1999). The relative error can be obtained with these theoretical data for every method (table 8).

Table 7: Theoretical data

t(d)	c/c_0	t(d)	c/c_0	t(d)	c/c_0	t(d)	c/c_0
0.1	0.057	0.25	0.691	0.4	0.943	0.55	0.991
0.15	0.259	0.3	0.891	0.45	0.967	0.6	0.995
0.2	0.5	0.35	0.898	0.5	0.983	0.65	0.997

Table 8: Calculation results of theoretical data

Name of method	DL(m^2/d)	relative error（%）
Method of breakthrough curves	0.564	12.8
Linear graphical method	0.507	1.4
Moment method	0.469	-6.2
Inverse function method	0.503	0.6

From table 8, it can be found that the relative error of four methods from small to big is respectively inverse function method, linear graphical method, moment method and method of breakthrough curves. In other words, the relative error of the commonly used method (method of breakthrough curves) is the biggest, although this method is easy to operate. Taking the result of inverse function method whose relative error is the smallest as reference, the close degree of results of other three methods relative to inverse function from small to big is respectively linear graphical method, moment method and break through.

According to this, the data in column 6 should be closer to data in column 13 than data in column 9 (Table 6). But this is not the case. In table1, the value of dispersion coefficient (DL) with moment method is closer to inverse function method than linear graphical method for data1, data3 and data5, and the value of DL with linear graphical method is closer to inverse function method than moment method for data2, data4 and average value.

Compared with the method of breakthrough curves, the relative error of the three methods mentioned in this paper is smaller when using theoretic data (Guo et al. 1997, 1997, 1999). The three methods avoid the errors caused by the subjective factors of artificial mapping and numerical reading, and the calculation results have high accuracy, but they have different applying conditions.

For linear graphical method, it can be found that yi is monotone decreasing function from expression (9). In order to guarantee that $T_{i+1/2}$ is meaningful in expression (10), value must be in the increasing trend. But the value of metrical fluctuate along with the time goes by. So the data which decrease with time must be deleted when using this method. Simultaneously, it must be guaranteed that the metrical time intervals of the rest data are more or less the same. Because the value yi varies with time, the value $y_{i+1/2}$ may become much larger relative to other value when the time interval is large. Much deviation of $y_{i+1/2}$ and $T_{i+1/2}$ may be caused under this situation mentioned before, which bring about the variety of DL. The consequence is that the waste of data resources and fluctuant results. Especially under the condition of that the metrical data itself is less and some data must be deleted, the results will change greatly. In a word, this method suits for the situation that plenty data, no fluctuation existing, and better linearity between $y_{i+1/2}$ and $T_{i+1/2}$.

The moment method needn't considerate the linearity compared with the other two methods. It can be completed via some simple calculation processes. Due to the fluctuation of measuring data have no effect on counting process. No data need to be deleted by this method. The relative error of theoretical data by using the moment method is smaller than that of by using the method of breakthrough curves, though there will be a little error among counting process when the difference quotient is used instead of the differential quotient. With inverse function method, it can be found that there is a good linear relationship between Gt and t. Show in figure 1 and 2. So it becomes unimportant whether the metrical data are more or less. And applying computer programming into the work of pegging normal function table will bring convenience. But the following situation must be noted. When the data are very small or close to 0.5, they must be deleted. Because inverse function value of y corresponding to these data will be very approximate or the same, and which will have great influence on the linearity of the results.

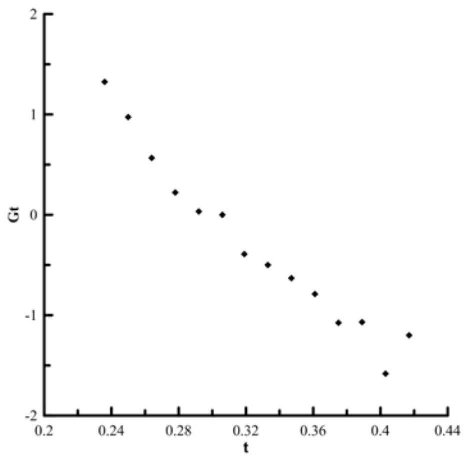

Figure 1: Inverse function method for data1

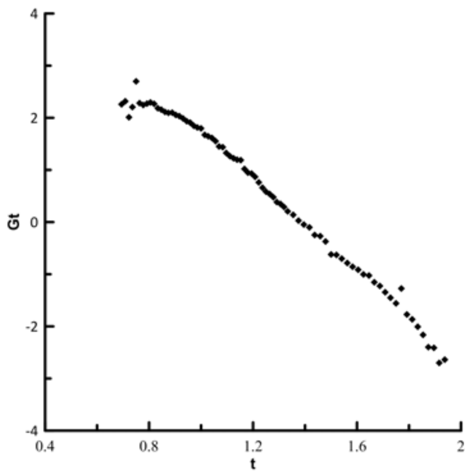

Figure 2: Inverse function method for data2

5. Conclusions

(1) With linear graphical method, the moment method and inverse function method, the dispersion coefficient in Yinchuan oil refinery are obtained. They are 0.068 m^2/d, 0.056 m^2/d and 0.081 m^2/d respectively. The three results are approximate. These methods avoid the errors caused by the subjective factors of artificial mapping and numerical reading. Data can be quickly and easily calculated by computer.

(2) For linear graphical method, the fluctuation and the interval of value have great effects on the results. Adding or deleting some data will also lead to the variety of results.

(3) Although the fluctuation of value has no effect on the moment method, this approximate calculation which the difference quotient is used instead of the differential quotient brings error to the results.

(4) The fluctuation, interval and quantity of data all have no influence on results with inverse function method. And the value of seepage velocity (V) didn't need to be known. So inverse function method is a decent method. However, as to the mountainous work of looking up the normal function table, computer programming brings convenience.

(5) Overall, it can be observed that the inverse function method is easy to calculate the dispersion coefficient under one-dimensional dispersion, which has less known conditions, smaller relative error and well linearity of results.

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