Text S1. Linear fitting formula for injection rate and time of each stage.
Stage 1.1 "q = −0.33t+11.39" k = −0.33
Stage 1.2 "q = −0.10t+10.99" k = −0.10
Stage 1.3 "q = −0.008t+10.5" k = −0.008
Stage 2 "q = −0.30t+16.36" k = −0.30

Text S2. The groundwater numerical simulation software groundwater model system (GMS) was used to simulate the seepage field of the experimental area.

The site can be generalized into a heterogeneous, isotropic, two-dimensional spatial structure unstable groundwater flow system, which can be described by the definite solution problem of the following partial differential equation。

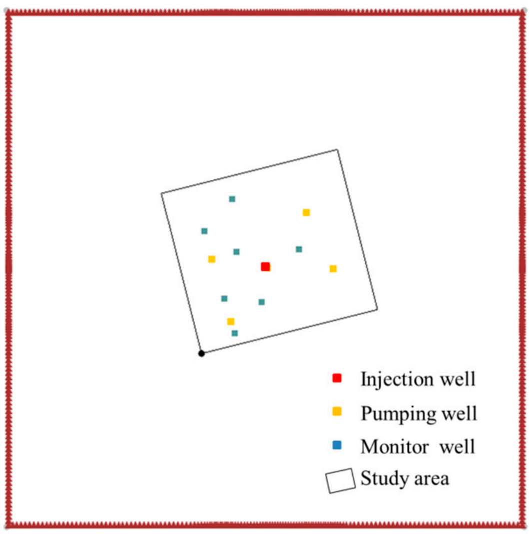
$$\mu_s \frac{\partial h}{\partial t}=\frac{\partial h}{\partial x}\left(K\frac{\partial h}{\partial x}\right)+\frac{\partial h}{\partial y}\left(K\frac{\partial h}{\partial y}\right)+W$$

$$h(x,\ y,\ t)=h_0(x,\ y) \qquad (x,\ y,\ z)\in\Omega,\ t=0$$

$$\frac{\partial h}{\partial n}+ah=b$$

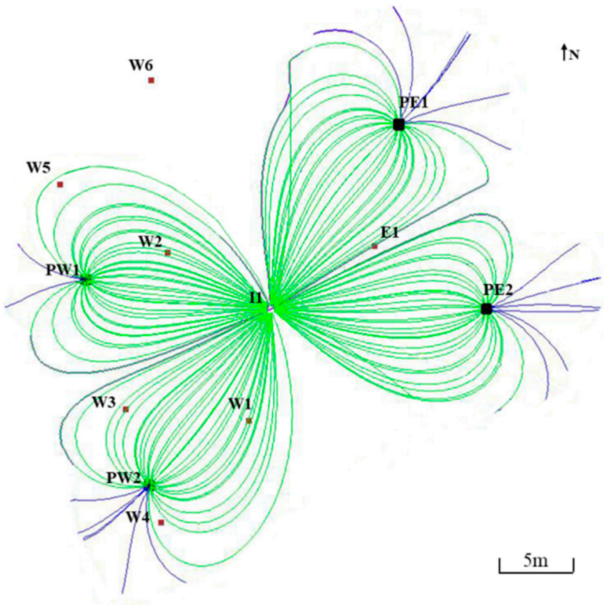
??$_s$$\mu_s$ is storativity (1/m), h is water level (m), K is permeability coefficient (m/d), t is time (d), W is source sink term(1/d), $h_0(x???y???z)$$h_0(x,y,z)$is known water level distribution, ??$\Omega$is the simulation area of the model.

Overview of the numerical model: The simulation range is 120 m long, 120 m wide, and has an area of about 14400 m^2. The experimental area is located in the center. The site is located in the desert with arid climate, very little precipitation, and deep water level, so the source and sink items are only for pumping water from pumping wells and injecting water from water injection wells. The aquifer is generalized as one layer with an average thickness of 25 m. The permeability coefficient of the entire simulation area is set to 3 m/d.



The numerical model range.

According to the established two-dimensional seepage model the flow field of the entire experimental area is obtained and then the envelope between each pumping well and water injection well, that is, the area of each equilibrium area is obtained according to the envelope. Acquire the length L of the water-passing section at each observation point according to the envelope.



Four equilibrium areas obtained from the numerical model.

Text S3. Calculation of Dispersion.

Taking the COD concentration $(C-C_{background})/(C_{injection}-C_{background})$ in the monitoring well as the ordinate axis and the corresponding time t as the abscissa axis the breakthrough curve was drawn. Find the time $t_{0.16}$, $t_{0.5}$, $t_{0.84}$ corresponding to $(C-C_{background})/(C_{injection}-C_{background}) = 0.16, 0.5, 0.84$ from the breakthrough curve and calculate according to the following formula [1]:

$$\alpha = \frac{D}{\mu}$$

$$\mu = \frac{L}{t_{0.5}}$$

$$D = \mu^2 \cdot (t_{0.84}-t_{0.16})^2/(8t_{0.5})$$

A is the dispersion (distance) (m)： μ is the actual migration velocity (m/d); *L* is the distance from monitor well to injection well (m), *D* is diffusion coefficient (m^2/d)。

Table S1. The breakthrough times of COD, H^+ and neutralization times obtained by fitting the C-t sequence with the Boltzmann function.

Monitor Wells	COD		H^+		Distance to injection well (m)	Neutralized time (d)
	t_{COD} (d)	R^2	t_H (d)	R^2		
W1	4.93	0.86	6.43	0.99	8	1.5
W2	5.71	0.96	7.42	0.99	8.2	1.71
W3	11.52	0.95	14.25	0.99	12.3	2.73
W4	17.03	0.9	23.11	0.91	16.6	6.08
W5	19.9	0.96	27.89	0.84	17.15	7.99
W6	21.82	0.98	28.04	0.99	18.2	6.22
E1	26.5	0.81	27.94	0.91	8.45	1.44

Table S2. Theoretical time of each section according to the numerical model.

		I1~W1					I1~W2		
S (m)	**H (m)**	**I**	**u_m (m/d)**	**t (d)**	**S (m)**	**H (m)**	**I**	**u_m (m/d)**	**t (d)**
0.36	27.25	—	—	—	0.42	27.25	—	—	—
2.00	26.32	0.47	6.42	0.32	2.05	26.47	0.38	5.25	0.39
4.00	25.94	0.19	2.62	0.78	4.10	25.84	0.31	4.24	0.48
6.00	25.68	0.13	1.79	1.14	6.15	25.64	0.10	1.35	1.52
8.00	25.50	0.09	1.24	1.65	8.20	25.48	0.08	1.08	1.90
Theoretical time (d)				**3.89**	**Theoretical time (d)**				4.30
		W1~W4					**W2~W5**		
S (m)	H (m)	I	u_m (m/d)	t (d)	S (m)	H (m)	I	u_m (m/d)	t (d)
8.00	25.50	—	—	—	8.20	25.48	—	—	—
10.15	25.30	0.10	1.38	1.49	10.45	25.32	0.08	1.08	2.09
12.30	25.19	0.05	0.74	2.78	12.70	25.20	0.06	0.81	2.79
14.45	25.10	0.04	0.62	3.33	14.95	25.10	0.05	0.67	3.34
16.60	25.03	0.04	0.53	3.88	17.20	25.02	0.04	0.54	4.18
Theoretical time (d)				11.49	Theoretical time (d)				12.39

Extract the water level data (H) of I1~W1~W4 and I1~W2~W5 from the numerical model and divide the water level data to obtain the hydraulic gradient ($I = \frac{\Delta H}{S}$) of each section. According to the original permeability coefficient K = 2.76m/d the migration velocity ($\mu_m = \frac{KI}{n}$)of each section was calculated and then the migration time ($t = \frac{S}{\mu_m}$)was obtained. The sum of time of each section was the theoretical migration time to a certain observation point.

Table S3. Actual migration velocity (μ) and permeability coefficient (K) after water injection of two sections in the same radial direction with different distances from the injection well.

Section	s (m)	t (d)	μ (m/d)	I	K (m/d)
I1~W1	8	4.93	1.62	0.22	1.48
W1~W4	8.6	12.1	0.71	0.05	2.59
I1~W2	8.2	5.71	1.44	0.22	1.33
W2~W5	9	14.19	0.63	0.05	2.48

S is the length of each section (m). Migration time (t) of each section is calculated according to breakthrough times of COD of each monitor well. Actual migration velocity $\mu = \frac{S}{t}$. Permeability coefficient ($K_i = \frac{\mu n}{I}$)after water injection of two sections in the same radial direction with different distances from the injection well were calculated according μ, I and porosity ($n = 0.2$).

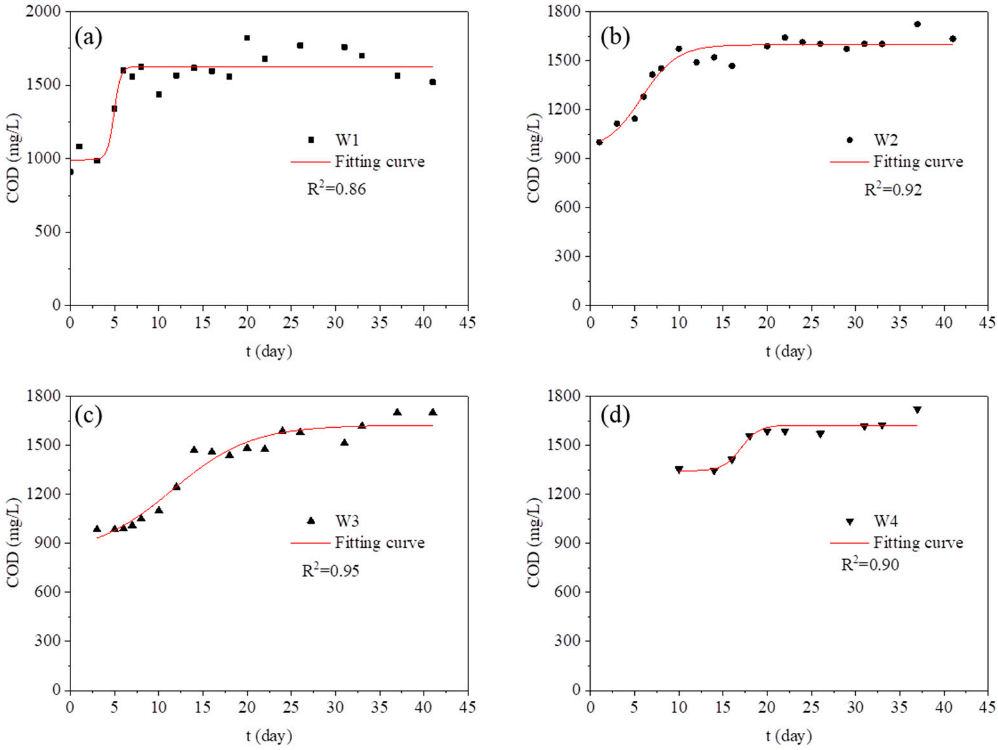
Table S4. Calculation of neutralized H^+ in each equilibrium area.

Equilibrium area	monitor well	t_{COD} (d)	t_{pH} (d)	S (m)	t_{ne} (d)	μ (m/d)	L (m)	C_a (mol)	q_n (mol)	q_n of quilibrium area (mol)
PW2	W1	4.93	6.43	8	1.5	1.62	10.14	3.16E-11	1.95	7.81
	W3	11.52	14.25	12.3	2.73	1.07	15.23	1.10E-10	3.51	
	W4	17.03	23.11	16.6	6.08	0.97	16.67	3.47E-11	7.81	
PW1	W2	5.71	7.42	8.2	1.71	1.44	10.05	1.00E-14	1.95	8.72
	W5	19.9	27.89	17.15	7.99	0.86	16.02	1.45E-11	8.72	
PE1	E1	26.5	27.94	8.45	1.44	1.44	8.95	3.72E-11	1.46	1.67
	PE1	30.4	31	15.7	0.6	2.37	14.88	1.00E-14	1.67	
PE2	PE2	29.5	33	15.1	3.5	1.31	14.37	3.98E-10	5.23	5.23

t_{ne},t_{COD},t_{pH} are neutralization time, breakthrough time of COD and pH respectively (d), μ is actual groundwater velocity (m/d), q_n is neutralized H^+ (mol), S is distance of monitor well to injection well (m); L is The length of the water-passing section at the observation well (m), the streamline of each equilibrium area is obtained by the numerical simulation, so as to acquire the length of the water-passing section, M is aquifer thickness (the thickness of the study area is 25m), n is porosity (0.2), C_I、C_a are the OH^- concentration of the injected water and the OH^- concentration when the observation well breakthrough, respectively (mol/L) (C_I = 3.16E-06).

Table S5. Dispersion at each observation well.

Monitor well / Param	W1	W4	W2	W5	W3
$t_{0.16}$	4.30	15.36	5.10	14.53	7.05
$t_{0.5}$	4.93	17.03	5.71	19.90	11.52
$t_{0.84}$	5.56	29.70	6.48	31.16	15.40
L (m)	8.00	16.60	8.20	17.15	12.30
μ (m/d)	1.62	0.71	1.44	0.63	1.07
D (m^2/d)	0.11	0.76	0.09	0.69	0.87
α (m)	0.07	1.07	0.06	1.09	0.81



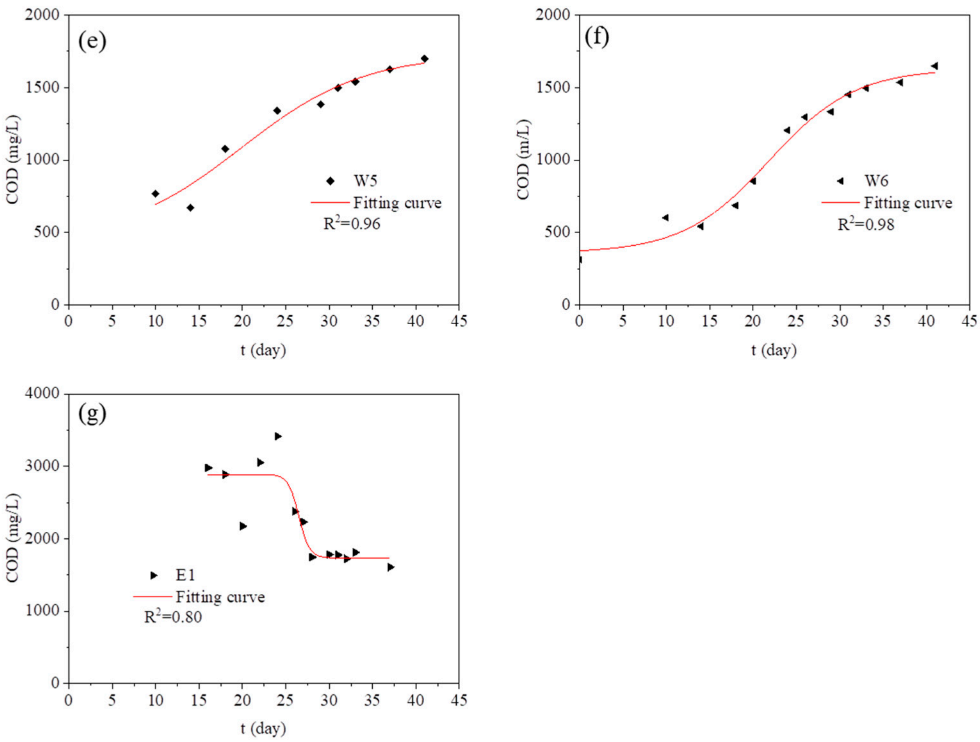
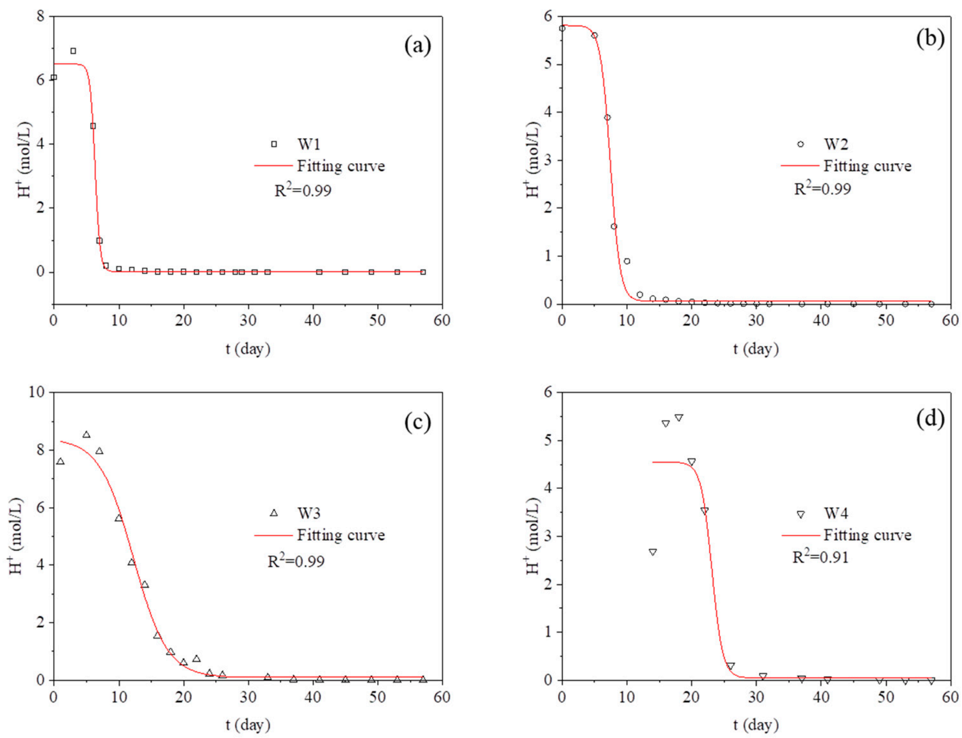


Figure S1. COD~t fitting curves of monitor wells W1~8 and E1 (a)~(g).



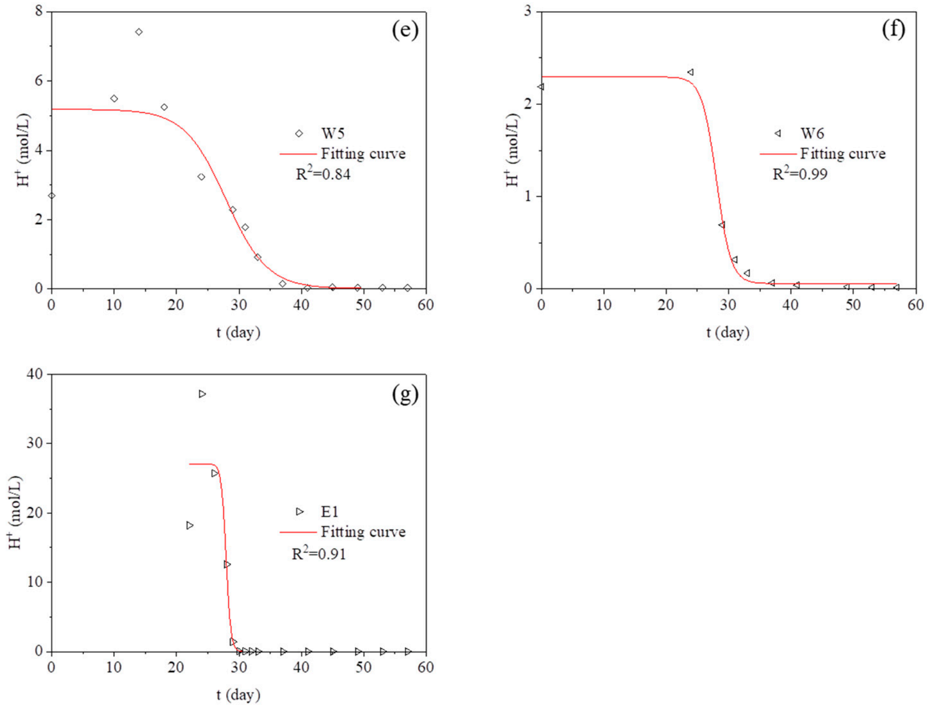


Figure S2. pH~t fitting curves of monitor wells W1~8 and E1 (a)~(g).

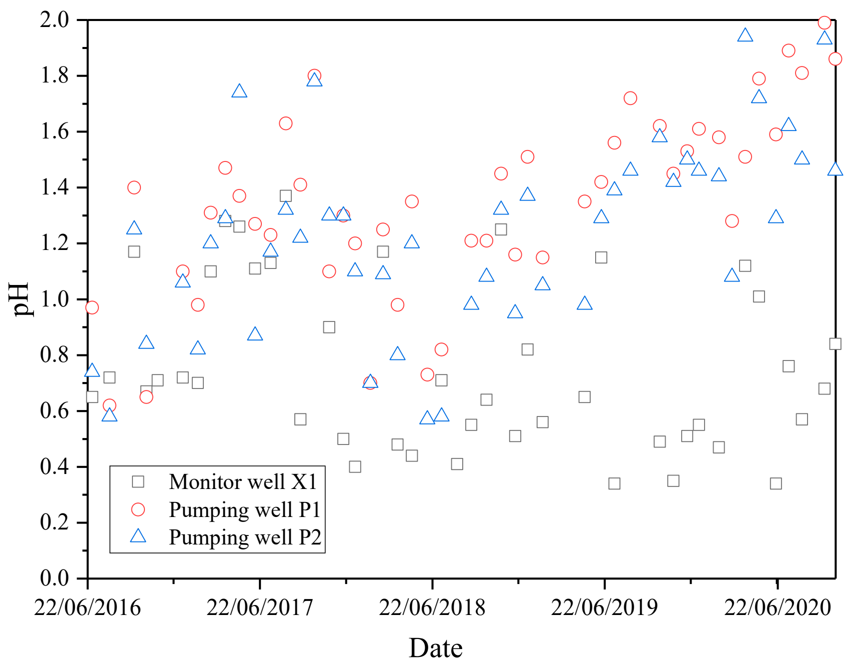


Figure S3. pH data of monitor well X1 and long-term pumping wells P1 and P2 in the site.

Reference

1. Bu X.F. and Wan W.F. Experimental Research on the Hydrodynamic Dispersion Characteristics of Loess Medium in Hilly Area of Western Henan Province. *China Rural Water and Hydropower* **2021**, *12*, 27–31.