function Equations\_by\_Zhongfu\_Wang %For time-dependent CA based GA model; Experimental data was abtained for oleic-acid coated glass beads in Figure (4);Please copy the total code to MATLAB and run it.

clear all;clc

format long

tspan=[0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350 360 370 380 390 400 410 420 430 440 450 460 470 480 490 500 510 520 530 540 550 560 570 580 590 600 610 620 630 640 650 660 670 680 690 700 710 720 730 740 750 760 770 780 790 800 810 820 830 840 850 860 870 880 890 900 910 920 930 940 950 960 970 980 990];%Measured Time

yexp=[0.011075481 0.022690826 0.032455056 0.041441214 0.050212894 0.058951298 0.065757891 0.072751079 0.08149635 0.087878941 0.094371946 0.102475836 0.108859679 0.115261668 0.12290134 0.128923351 0.135391055 0.142244948 0.148339372 0.155038107 0.161286129 0.167646918 0.174145957 0.179922405 0.186415332 0.192082842 0.198176362 0.204381551 0.210420203 0.21645139 0.222200332 0.228148636 0.233768759 0.239450313 0.245289686 0.250993891 0.256885891 0.262542114 0.268481635 0.274198842 0.279911297 0.285648755 0.291149478 0.296750074 0.302213317 0.307860061 0.313373158 0.319019105 0.324518466 0.33007712 0.33560058 0.341294085 0.34687305 0.35241363 0.357936938 0.363419012 0.368918445 0.374521197 0.37969101 0.385347429 0.390546897 0.396224253 0.401374682 0.407136311 0.412256578 0.418007641 0.423023901 0.428823515 0.433754245 0.439607234 0.444520239 0.45034023 0.455286023 0.46109649 0.466105947 0.471889933 0.476871294 0.482512757 0.48764997 0.493488755 0.498379117 0.503989632 0.508955372 0.514563132 0.519634398 0.525072469 0.530293933 0.53566845 0.540870877 0.546118047 0.551420145 0.556680744 0.56192702 0.566976549 0.572494564 0.577456601 0.583067317 0.587854457 0.593487028]';%Measured wetting front position

ml=[0 0.011075481 0.022690826 0.032455056 0.041441214 0.050212894 0.058951298 0.065757891 0.072751079 0.08149635 0.087878941 0.094371946 0.102475836 0.108859679 0.115261668 0.12290134 0.128923351 0.135391055 0.142244948 0.148339372 0.155038107 0.161286129 0.167646918 0.174145957 0.179922405 0.186415332 0.192082842 0.198176362 0.204381551 0.210420203 0.21645139 0.222200332 0.228148636 0.233768759 0.239450313 0.245289686 0.250993891 0.256885891 0.262542114 0.268481635 0.274198842 0.279911297 0.285648755 0.291149478 0.296750074 0.302213317 0.307860061 0.313373158 0.319019105 0.324518466 0.33007712 0.33560058 0.341294085 0.34687305 0.35241363 0.357936938 0.363419012 0.368918445 0.374521197 0.37969101 0.385347429 0.390546897 0.396224253 0.401374682 0.407136311 0.412256578 0.418007641 0.423023901 0.428823515 0.433754245 0.439607234 0.444520239 0.45034023 0.455286023 0.46109649 0.466105947 0.471889933 0.476871294 0.482512757 0.48764997 0.493488755 0.498379117 0.503989632 0.508955372 0.514563132 0.519634398 0.525072469 0.530293933 0.53566845 0.540870877 0.546118047 0.551420145 0.556680744 0.56192702 0.566976549 0.572494564 0.577456601 0.583067317 0.587854457 0.593487028];%Measured wetting front position

mql=[0 4.69095E-06 8.9673E-06 1.12458E-05 1.36023E-05 1.62523E-05 1.6932E-05 1.67645E-05 2.11683E-05 2.27959E-05 2.09229E-05 2.54707E-05 2.74457E-05 2.5733E-05 2.99235E-05 3.10429E-05 2.97526E-05 3.33447E-05 3.40607E-05 3.50736E-05 3.71084E-05 3.75883E-05 3.98534E-05 3.95295E-05 4.08042E-05 4.19079E-05 4.17481E-05 4.50559E-05 4.62567E-05 4.69498E-05 4.71438E-05 4.80518E-05 4.87971E-05 4.88302E-05 5.1E-05 5.23375E-05 5.38043E-05 5.48325E-05 5.6278E-05 5.78569E-05 5.79368E-05 5.92484E-05 5.93533E-05 5.97523E-05 6.06923E-05 6.20695E-05 6.35069E-05 6.46442E-05 6.57221E-05 6.63369E-05 6.76145E-05 6.95924E-05 7.11199E-05 7.13078E-05 7.20774E-05 7.28272E-05 7.37762E-05 7.57158E-05 7.45816E-05 7.6001E-05 7.73333E-05 7.85386E-05 7.93093E-05 8.0984E-05 8.1907E-05 8.28653E-05 8.32038E-05 8.4591E-05 8.50646E-05 8.64824E-05 8.75028E-05 8.82134E-05 8.96428E-05 9.05484E-05 9.22469E-05 9.30125E-05 9.39311E-05 9.36706E-05 9.61698E-05 9.89729E-05 9.79001E-05 9.67534E-05 9.85636E-05 9.94946E-05 0.000101601 0.000100965 0.000103493 0.000103887 0.000104767 0.000104494 0.000106529 0.000107703 0.000108158 0.000106989 0.000110793 0.000110927 0.000112893 0.000112102 0.000113268 0.000111254];%Measure Darcy velocity\*wetting front position

k0=[-0.752855123858705 0.000181035563809658 -0.118086424926025 0.00536854016023314 0.000247782528309054 523.046616568686]; %Initial values were obtained from 1stOpt software. For more details, please refer to the Materials and Methods part in the paper

t0=0;

yp0=0;

y0=0.0000000001; %y0 was set as 10^-10 to initiate computation

lb=-[0 0 0.1 0.01 -0.0001628 -87.5]; %Lower boundary

ub=[0.38 0.000009 -0.04 -0.00996 0.0001632 87.51];%Upper boundary

yy=[y0 yexp'];

[k,resnorm,residual,exitflag,output,lambda,jacobian] = ...

lsqnonlin(@ObjFunc,k0,lb,ub,[],tspan,y0,yexp);

fprintf('\n\nUsing lsqnonlin()get follwing parameter:\n')

fprintf('\t k1 = %.6f\n',k(1))

fprintf('\t k2 = %.6f\n',k(2))

fprintf('\t k3 = %.6f\n',k(3))

fprintf('\t k4 = %.6f\n',k(4))

fprintf('\t k5 = %.6f\n',k(5))

fprintf('\t k6 = %.6f\n',k(6))

ts=0:0.01:max(tspan);

[y0,yp0] = decic(@Equations,t0,y0,1,yp0,0,[],k);

[ts ys]=ode15i(@Equations,ts,y0,yp0,[],k); %Ode15i was used to solve implicit differential equation

m=gradient(ys)./gradient(ts);

subplot(1,2,1)

plot(ml,mql,'dk','LineWidth',1.2)

hold on

plot(ys,m\*0.369.\*ys,'m','LineWidth',2)

legend('Oleic-acid coated glass beads', 'Calculated by equation (8)','Location','best');

xlabel('l [m]')

ylabel('ql [m^2/s]')

subplot(1,2,2)

plot(tspan,yy,'dk','LineWidth',1.2)

hold on

plot(ts,ys,'m','LineWidth',2)

legend('Oleic-acid coated glass beads','Calculated by equation (8)','Location','best');

xlabel('t [s]')

ylabel('l [m]')

%Small figure

%%Line 48-54 to get fitted time-dependent suction head.

axes('Position',[0.62,0.615,0.14,0.14]);

syms x

x=0:0.1:1000

y=((0.19\*exp(0.000005\*x)-0.070\*exp(-0.009980\*x)))

plot(x,y,'-m','LineWidth',2)

xlabel('t [s]')

ylabel('Suction head [m]')

%---------------------------------------------------------

function f = ObjFunc(k,tspan,y0,yexp) %Objective function was formulated for ql VS. l

t0=0;

yp0=0;

[y0,yp0] = decic(@Equations,t0,y0,1,yp0,0,[],k); %Compute consistent initial conditions for ode15i

[t Xsim] = ode15i(@Equations,tspan,y0,yp0,[],k);

n=gradient(Xsim)./gradient(t);

nsim=n(2:end)

ysim = Xsim(2:end);

size(nsim);

size(ysim);

size(yexp);

mq=[0.000419728 0.000395153 0.000346429 0.000327976 0.000323724 0.000287415 0.000254932 0.000290901 0.000279592 0.000237925 0.000269813 0.000267772 0.00023631 0.000259524 0.000252466 0.000231037 0.000246259 0.000239201 0.000236565 0.000239286 0.000233163 0.000237755 0.000226786 0.000226871 0.000224745 0.000217517 0.000227381 0.000226361 0.000223129 0.000217687 0.000216241 0.000213776 0.000209014 0.000212925 0.000213435 0.000214371 0.00021352 0.000214371 0.000215476 0.00021131 0.00021165 0.000207738 0.000205187 0.000204592 0.000205357 0.000206378 0.000206293 0.000206122 0.000204422 0.000204932 0.000207398 0.000208418 0.000205612 0.000204592 0.000203486 0.000203061 0.000205272 0.00019915 0.00020017 0.00020068 0.000201105 0.00020017 0.000201786 0.00020119 0.00020102 0.000199065 0.0002 0.000198384 0.000199405 0.000199065 0.000198469 0.000199065 0.000198895 0.000200085 0.000199575 0.000199065 0.000196429 0.00019932 0.000202976 0.000198384 0.000194133 0.000195578 0.000195493 0.000197449 0.000194303 0.000197109 0.000195918 0.000195578 0.000193197 0.000195068 0.000195323 0.000194303 0.000190391 0.000195408 0.000193793 0.000195493 0.000192262 0.000192687 0.0001875]';

size(mq)

f=nsim.\*0.369.\*ysim-yexp.\*mq;

%----------------------------------------------------------

function res = Equations(t,y,yp,k)

beta(1)=k(1); %a in time-dependent suction head function

beta(2)=k(2); %b in time-dependent suction head function

beta(3)=k(3); %c in time-dependent suction head function

beta(4)=k(4); %d in time-dependent suction head function

beta(5)=k(5); %K saturated hydraulic conductivity

beta(6)=k(6); %Lumped number

res = (((beta(1)\*exp(beta(2)\*t)+beta(3)\*exp(+beta(4)\*t)))+0.03-(0.07051\*beta(6)/(1.466))\*((0.01476)\*yp).^(0.3)+y)\*(beta(5)/0.369)/(y)-yp;