

The following scripts is under the license Creative Commons Attribution 4.0 International license



```
%% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%  
%% ----- MORFEO HC v. 1.0 ----- %%  
%% ---- Monte Carlo Simulation Ramirez Fons for Half Cell ----- %%  
%% -----Diffusion Experiment Evaluation and Optimization ----- %%  
%% ----- %%  
%% PartI: Determination of minimum evolved region for Half-Cell experiments %%  
%% ----- Creative Commons cc by ----- %%  
%% ----- Jordi Fons & Oriol Ramirez ----- %%  
%% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
%% DESCRIPTION AND GUIDE FOR USERS
```

```
% This script simulates non evolved half-cell diffusion experiments and fit  
% the simulated data to an error function to obtain diffusion profiles in  
% order to evaluate the minimum evolved region necessary to ensure the  
% contribution of migration in the evolved region observed. The key  
% parameters considered are the variability in the activity concentration of  
% both plugs, the non-infinitesimal sliced of the plug (due to the particle  
% size of the sample analysed) and its variability.
```

```
% It is recommended just to modify the input data to adjust the simulation  
% to the specific experimental conditions. Any modification of the simulation  
% section may lead to a loss of functionality of the script.
```

```
clear  
close
```

```
%% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% INPUT DATA %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% %%  
%-----%
```

```
repeticionsacom=50; % Number of non-evolved diffusion tubes simulated  
nacom=8000; % Number of point used to simulate one diffusion tube  
ndacom=80; % Length of the diffusion tube in mm  
ACBacom=95; % Activity concentration of the low activity plug  
ACAacom=4800; % Activity concentration of the high activity plug  
sAacom=0.1; % Relative Standard Deviation (RSD) of low and high activity  
%concentration  
cmmacom=0.000000001; % evolved region in mm, 0.000000001 for non-evolved  
sacom=2; % mean distance between slices in mm  
rsdsacom=0.3; % RSD in the distance between slices  
numacom=10; % Number of slices in the plateaus (plug ends) used to calculate  
%the mean value for each plateau  
%-----%
```

```
%% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% SIMULATION %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% %%  
% -- Following section should not be modified unless users-----%  
%----want to adapt the script for simulating diffusion experiments-----%  
%-----of set-ups other than half-cell-----%  
%% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
repacom=1;  
while repacom<repeticionsacom+1;
```

```

clearvars -except -regexp acom$; %Delete all the variables except the ones
% needed to save the results.

% Variable definition
n=nacom;
nd=ndacom;
ACB=ACBacom;
sA=sAacom;
ACA=ACAacom;
cmm=cmmacom;
c=(n/nd)*cmm;
pmm=n/nd;
s=sacom;
rsds=rsdsacom;
sds=s*rsds;
mpps=pmm*s;
sdpps=pmm*rsds;
num=numacom;

%% SIMULATION OF THE DIFFUSION TUBE
%% Generate a sigmoid curve from -n/2 to n/2 with the input evolved region(c)
distp=[(-1*n/2):1:(n/2)]';
actn=erf((distp)/(c));
AM=(ACA+ACB)/2; % Mean activity in the tube
ci=(ACA-AM)*actn+AM;
%% Include the input dispersion in the generated points to simulate the
%% dispersion between slices
si=ci*sA*sqrt((n)/((n/80)/sA)); %SD as a function of the activity
aleat=randn(1,n+1); %Generates n+1 random numbers following a normal
%distribution with a mean value of 0 and standard deviation of 1
i=1;
while i<length(si)+1
    cdi(i)=ci(i)+si(i).*aleat(i);
    i=i+1;
end

%% Slices Generator (generates randomly slices with width "s" (in mm)
% and a RSD of "rsds"

slicepunts=0;
i=1;
while sum(slicepunts)<n;
    slicepunts(i)=round(mpps+sdpps.*randn(1,1));
    i=i+1;
end
uslice=sum(slicepunts)-n;
% Modify the width of the last slices to ensure that all simulated tubes
% have a 80mm-length
if uslice > mpps/2;
    slicepunts(i-2)=nacom-sum(slicepunts(1:i-3));
    numslices=i-2;
else
    slicepunts(i-1)=nacom-sum(slicepunts(1:i-2));
    numslices=i-1;
end
slicep=slicepunts(1:numslices);
%% Define the vector with the distance between slices in mm
i=1;
j=0;
distac(1)=slicep(1);

```

```

while i<numslices+1;
    dist(i)=(2*j+slicep(i))/2;
    distac(i+1)=distac(i)+slicep(i);
    j=j+slicep(i);
    i=i+1;
end
dist=dist';
distac=distac-distac(1);
distac=distac';
%% Calculate the activity concnetration for each slice
act=zeros((numslices),1);
k=1; %Each slice
l=1; %Each point-activity inside the vector ci
while k<numslices+1 %For each slice
    o=1; % number of point inside the slice
    while o<(slicep(k))+1; % For all the points in the slice
        act(k)=act(k)+cdi(l);
        o=o+1;
        l=l+1;
    end
    k=k+1;
end
%% Calculate the concentration activity for each slice
k=1; %Each slice
while k<numslices+1;
    act(k)=act(k)/slicep(k);
    k=k+1;
end

%% DIFFUSION TUBE SIMULATED
%% Output data:

distac;          % % % % % % % % % % % % % % % % % % % % % % %
dist;            % distac = End of each slice in points      %
act;             % dist = Centre of each slice in points     %
                % act = Activity concentration of each slice %
                % % % % % % % % % % % % % % % % % % % % % % %

%% NORMALIZATION OF THE SIMULATED TUBE
% Activity
    mbaix=mean(act(1:num));
    malt=mean(act(end-num:end));
    mitja=(mbaix+malt)/2;
    actn=(act-mitja)/(malt-(mitja));
    % Warning!! in some Matlab versions it can not work due to "act" is a
    % vector and "mitja" and "malt" are scalars. It can be modified to:
    % actn(:,1)=(act(:,1)-mitja)/(malt-(mitja))
% Position
    distc=(dist-(n/2))*nd/n; %Recalculate the position considering 0 the
    % contact surface between teo plugs

%% DIFFUSION TUBE NORMALIZED
%% Output data:

actn;            % % % % % % % % % % % % % % % % % % % % % % %
distc;           %          act = Normalized activity for each slice %
                %          distc= Centre of each slices normalized to 0 in mm %
                % % % % % % % % % % % % % % % % % % % % % % %

```



```

        plot ([distac(i)/100;distac(i)/100],[min(act);max(act)], 'k:')
        i=i+1;
    end

%% Plot 2
% Fittings for real and ideal data
figure(2)
axes('FontSize',14)
plot (distp/100+40, ((ACA-AM)*erf((distp)/(cmm*100)))+AM, 'b-', 'LineWidth',1)
hold on
plot(distp/100+40, actfitnorm, 'r:', 'LineWidth',1)
xlabel('Distance in mm', 'FontWeight', 'bold', 'FontSize',14)
ylabel('Activity concentration in Bq kg-1',...
        'FontWeight', 'bold', 'FontSize',14)
legend('Ideal data fitting', 'Real data fitting', 'location', 'Northwest')

% Zoom in the region of interest
figure (21)
axes('FontSize',14)
plot (distp/100+40, ((ACA-AM)*erf((distp)/(cmm*100)))+AM, 'b-', 'LineWidth',1)
hold on
plot(distp/100+40, actfitnorm, 'r:', 'LineWidth',1)
xlabel('Distance in mm', 'FontWeight', 'bold', 'FontSize',14)
ylabel('Activity concentration in Bq kg-1',...
        'FontWeight', 'bold', 'FontSize',14)
axis([37.5 42.5 0 5000])
legend('Ideal data fitting', 'Real data fitting', 'location', 'Northwest')

%% Plot 3
% Slices, with its activity and fitted function together with the
% residuals for each slice

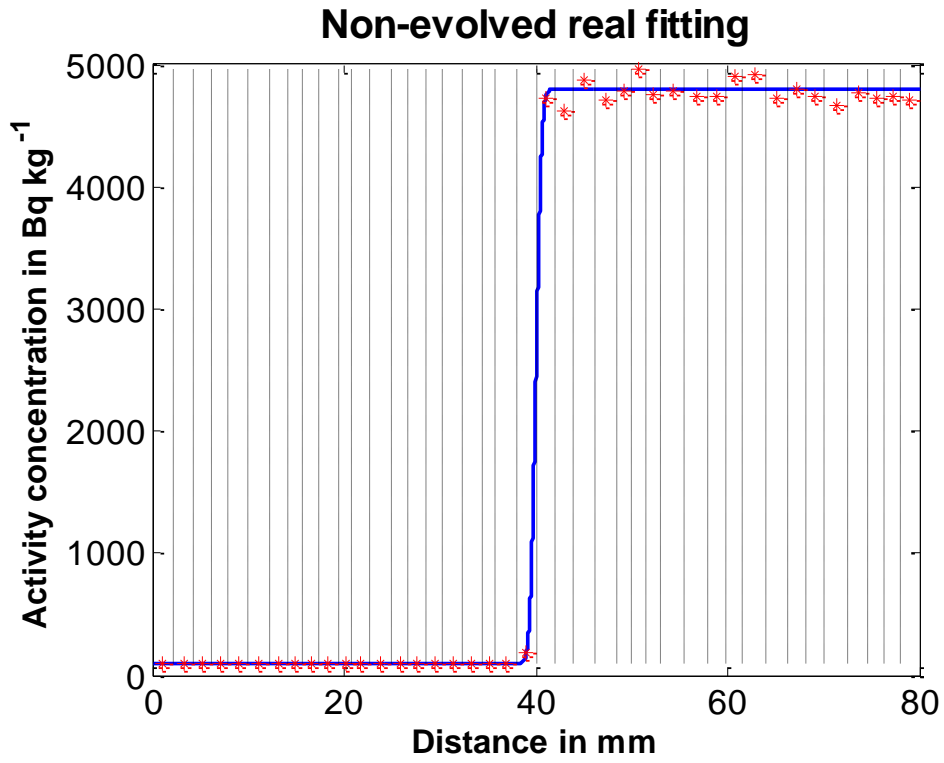
actfitada=erf(distp/(c*100));
actfitnorm= ((ACA-AM)*actfitada)+AM;
figure(3)
subplot(2,1,1)
plot(distp/100+40, actfitnorm, 'b-', 'LineWidth',2)
title('Fitting', 'FontSize',12, 'FontWeight', 'bold')
hold on
plot (distc+40,act, 'r*')
legend('Fitting', 'Act. Slices', 'location', 'SouthEast')
i=1;
xlabel('Distance in mm', 'FontWeight', 'bold', 'FontSize',10)
ylabel('Activity concentration in Bq kg-1',...
        'FontWeight', 'bold', 'FontSize',10)

while i<numslices+1
    plot ([distac(i)/100;distac(i)/100],[ACA;ACB], 'k:')
    i=i+1;
end
subplot(2,1,2)
plot(distc+40,residuals, 'r')
title('Residuals', 'FontSize',12, 'FontWeight', 'bold')
hold on
plot(distc+40,residuals, 'ko', 'MarkerSize',3)
xlabel('Distance in mm', 'FontWeight', 'bold', 'FontSize',10)

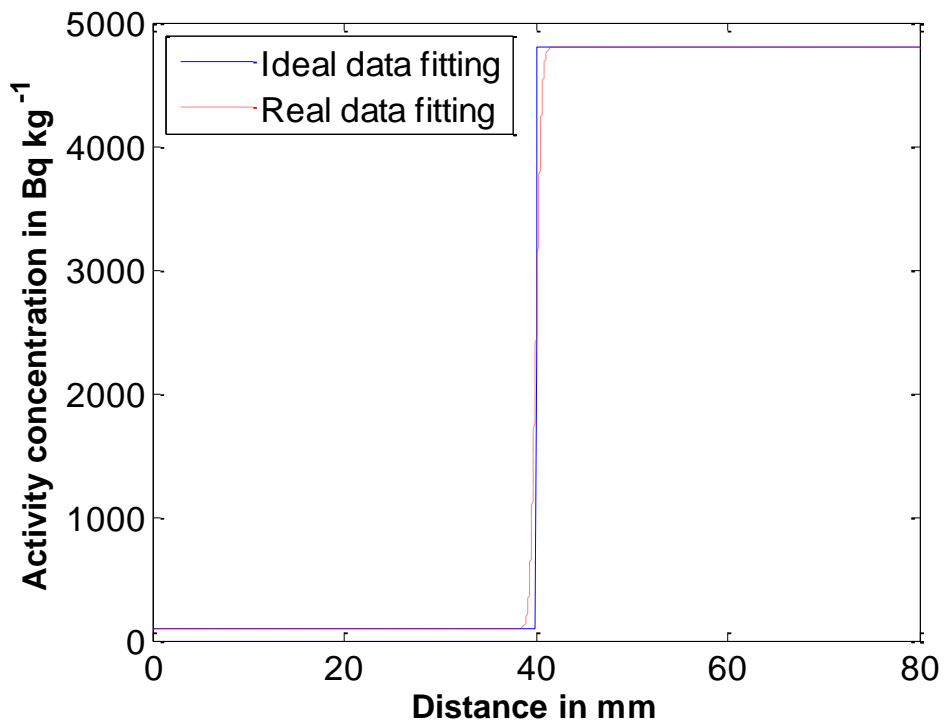
```

```
%% IMAGES
```

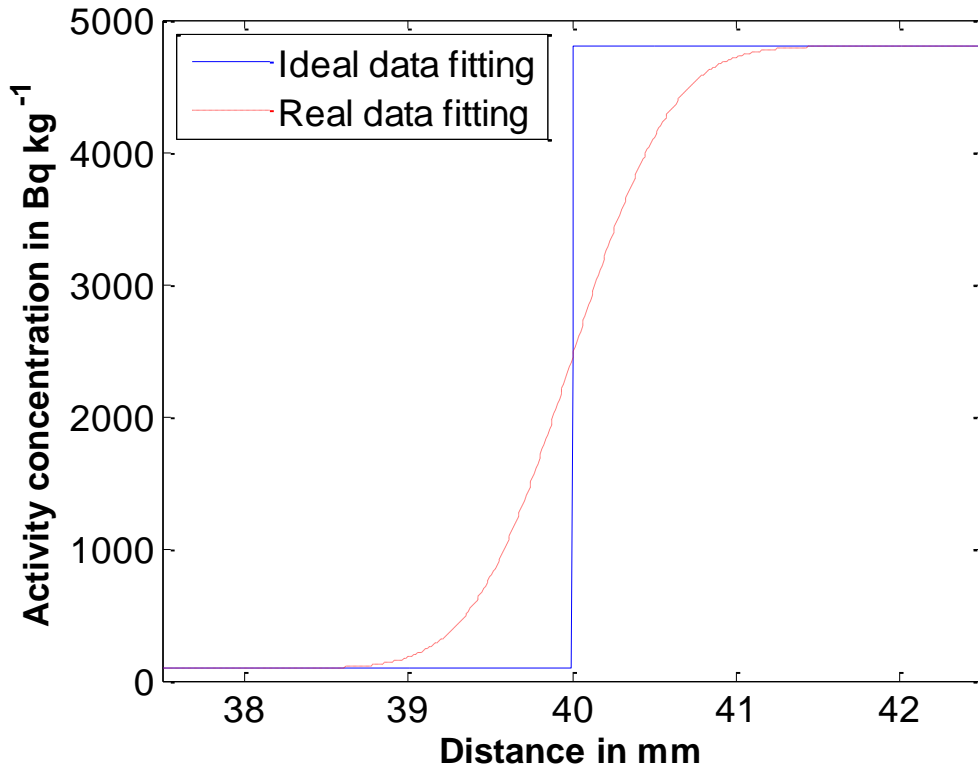
```
%% Plot 1
```



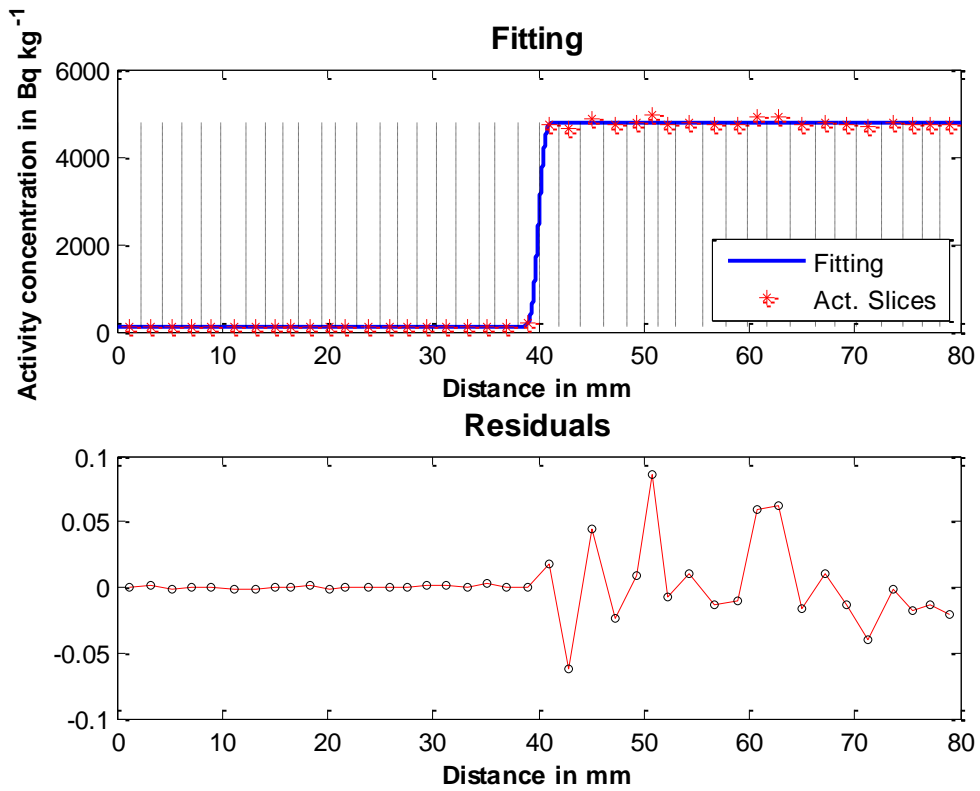
```
%% Plot 2
```



%% Plot 2 (Zoom)



%% Plot 3




```

%% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% %%
%% ----- MORFEO HC v. 1.0 ----- %%
%% ---- Monte Carlo Simulation Ramirez Fons for Half Cell ----- %%
%% -----Diffusion Experiment Evaluation and Optimization ----- %%
%% ----- %%
%% -- PART II: Determination of correction factor and uncertainty --- %%
%% ----- in Half-Cell experiments ----- %%
%% ----- Creative Commons cc by ----- %%
%% ----- Jordi Fons & Oriol Ramirez ----- %%
%% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% %%

```

```

%% DESCRIPTION AND GUIDE FOR USERS %%

```

```

% This script simulates evolved half-cell diffusion experiments and fit
% the simulated data to an error function to obtain diffusion profiles in
% order to evaluate the bias between fitted real profile and the real
% evolution of the diffusion tube. The parameters considered are the
% variability in the activity concentration of both plugs, the
% non-infinitesimal sliced of the plug (due to the particle size of the
% sample analyzed) and its variability.

```

```

% In this script, evolved diffusion profiles from 1 mm to 40 mm by
% progressing 1 mm at time, were simulated (200 profiles for each grade
% of evolution). This profiles, with a known evolution (ideal profiles),
% were treated in the same way that experimental profiles obtaining a
% fitted evolution (real profiles). In this way, the correction factor to
% correct fitted data into the evolution of the diffusion tube and its
% uncertainty were obtained.

```

```

% It is recommended just to modify the input data to adjust the
% simulation to the specific experimental conditions. Any modification of
% the simulation section may lead to a loss of functionality of the
% script.

```

```

% Input data in this script is divided in several sections for
% operational reasons.

```

```

clear
close
tic

```

```

%% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% INPUT DATA %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

```

```

%%
%-----
%
cmmxacom=1; % Minimum value of c simulated in mm
cmaxacom=40; % Maximum value of c simulated in mm
repeticionsxacom=200; % Number of diffusion tubes simulated for each c
%-----

```

```

calculsxacom=0;% Accountant
while cmmxacom<=cmaxacom % For each c
clearvars -except -regexp xacom$; % Delete variables from previous
%simulations of different c

```

```

repacom=1;
while repacom<repeticionsxacom+1; % For each tube

clearvars -except -regexp acom$; %% Delete variables from previous
%simulations of different tube

%% INPUT DATA
%%
%-----
%
n=8000; % Number of point used to simulate one diffusion tube
nd=80; % Length of the diffusion tube in mm
ACB=95; % Activity of the low activity plug
sA=0.05; % Relative Standard Deviation of ***
ACA=4800; % Activity of the high activity plug
s=2; % mean distance between slices in mm
rsds=0.3; % RSD in the distance between slices
num=10; % Number of slices in the plateaus used to calculate the mean
% value for each plateau

%-----
%

% Variable definition
cmmi=0.1;

cmm=cmmi+(cmmxacom-1)/10; %value of c in mm
c=(n/nd)*cmm; %value of c in points
pmm=n/nd; %points per mm
sds=s*rsds;
mpps=pmm*s;
sdpps=pmm*rsds;

%% SIMULATION OF THE DIFFUSION TUBE
%% Generate a sigmoid curve from -n/2 to n/2 with the input evolved
region(c)
    distp=[(-1*n/2):1:(n/2)]';
    actn=erf((distp)/(c));
    AM=(ACA+ACB)/2; % Mean activity in the tube
    ci=((ACA-AM)*actn)+AM;
%% Include the input dispersion in the generated points to simulate the
%% dispersion between slices
    si=ci*sA*sqrt((n)/((n/80)/sA)); %SD as a function of the activity
    aleat=randn(1,n+1); %Generates n+1 random numbers following a normal
    %distribution with a mean value of 0 and standard deviation of 1
    i=1;
    while i<length(si)+1
        cdi(i)=ci(i)+si(i).*aleat(i);
        i=i+1;
    end

%% Slices Generator (generates randomly slices with width "s" (in mm)
% and a RSD of "rsds"

```



```

Desvxacom (cmmxacom)=std(Cacom); % SD in "real" c for each "ideal" c
cmmxacom=cmmxacom+1
end
toc
%% %%%%%%%%%%% END OF THE SIMULATION %%%%%%%%%%% %%

%-----%

%% %%%%%%%%%%% RESULTS %%%%%%%%%%% %%

%% Check results
if calculsxacom==cmaxacom*repeticionsxacom
disp(' OK ')
else
disp('Warning!! Error in repetitions or on results accumulation')
end
%% Simulated data treatment
Cxacom; % mean of "real" c for each "ideal" c
Desvxacom; % SD in "real" c for each "ideal" c
Desvestacom=(Desvxacom./Cxacom); % RSD in "real" c for each "ideal" c
csimulades=cmmi:0.1:cmmi+(cmaxacom-1)/10; % c simulated
errorc=(Cxacom-csimulades)./csimulades*100; % Bias in C between "real" %
and "ideal"
toc

%% %%%%%%%%%%% REPRESENTATION OF THE RESULTS %%%%%%%%%%% %%

%% PLOT 1

MER=1.26 % Minimum Evolved Region (it can be calculated using MORFEO_HC
part I
% The data is fitted from MER to maximum C simulated
% -----
% Calculations
Cplus=Cxacom+Desvxacom;
Cminus=Cxacom-Desvxacom;
mer=round(MER*10)

opcions = fitoptions('Method','NonlinearLeastSquares',...
'Lower',0,...
'Upper',Inf,...
'StartPoint',1,...
'Robust','Bisquare');

funcio = fit(Cxacom(mer:end)',csimulades(mer:end)','poly2');
funciop = fit(Cplus(mer:end)',csimulades(mer:end)','poly2');
funciom = fit(Cminus(mer:end)',csimulades(mer:end)','poly2');

figure(1)
axes('FontSize',10)
hold on
plot(Cxacom,[csimulades],'b.')% Cideal vs real
plot(Cplus,[csimulades],'r.')
plot(csimulades(mer:end),funcio(csimulades(mer:end)),'b-','Linewidth',1)

```

```

%fitted Cideal vs real
plot(csimulades(mer:end),funciop(csimulades(mer:end)),'r-','Linewidth',1)
%fitted 95 % Cideal vs real
plot([0,cmmi+cmaxacom/10],[0,cmmi+cmaxacom/10],'k','Linewidth',1.5)
%Ideal correlation (ideal = real)
plot([MER MER],[0 MER+1.8],'k:','Linewidth',1.5)
plot(Cminus,[csimulades],'r.')
plot(csimulades(mer:end),funciom(csimulades(mer:end)),'r-','Linewidth',1)
%fitted 5 % Cideal vs real
ylabel('W from ideal profile in mm','FontWeight','bold','FontSize',12)
xlabel('W from real profile in mm','FontWeight','bold','FontSize',12)
legend('W_{real} vs W_{ideal}','5% and 95% for each W simulated',...
'Fitted curve W_{real} vs W_{ideal}','5% and 95% fitted curves',...
'Ideal correlation W_{real} = W_{ideal}','location','Southeast')
text(0.2,3.75, strcat('W_{ideal} = ',num2str(1000*funcio.p1/1000),...
' W_{real}^2 + ',num2str(1000*funcio.p2/1000),...
' W_{real} ',num2str(1000*funcio.p3/1000)), 'FontSize',10)
text(0.2,4.20, strcat('W_{ideal} { 95^{th}} = ',...
num2str(1000*funciop.p1/1000), ' W_{real}^2 + ',...
num2str(1000*funciop.p2/1000), ' W_{real} ',...
num2str(1000*funciop.p3/1000)), 'FontSize',10)
text(0.2,3.30, strcat('W_{ideal} { 5^{th}} = ',...
num2str(1000*funciom.p1/1000), ' W_{real}^2 + ',...
num2str(1000*funciom.p2/1000), ' W_{real} ',...
num2str(1000*funciom.p3/1000)), 'FontSize',10)
text(MER+0.05,MER+1.3, strcat('W_{min real}'),'FontWeight','bold',...
'FontSize',10)

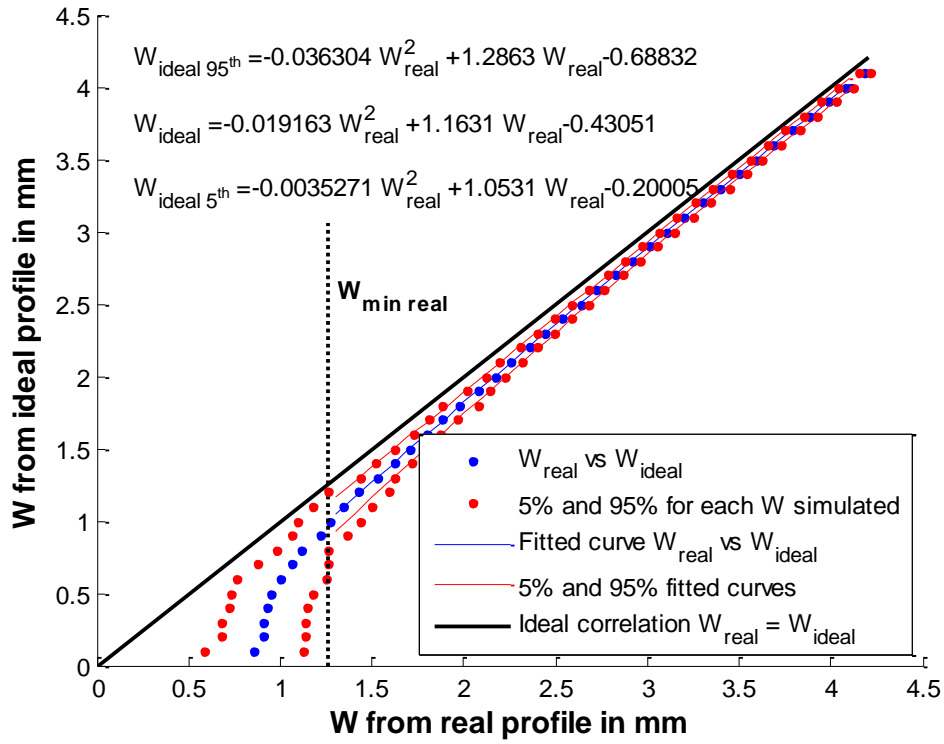
%% PLOT 2

% Bias between real and ideal evolved profiles
figure (21)
axes('FontSize',12)
plot (csimulades, errorc)
hold on
plot([MER MER],[0 500],'k:','Linewidth',1.5)
xlabel('W from ideal profile in mm','FontWeight','bold','FontSize',12)
ylabel('% of bias between real and ideal
profiles','FontWeight','bold',...
'FontSize',12)
text(MER+0.05,450, strcat('W_{min}'),'FontWeight','bold','FontSize',10)

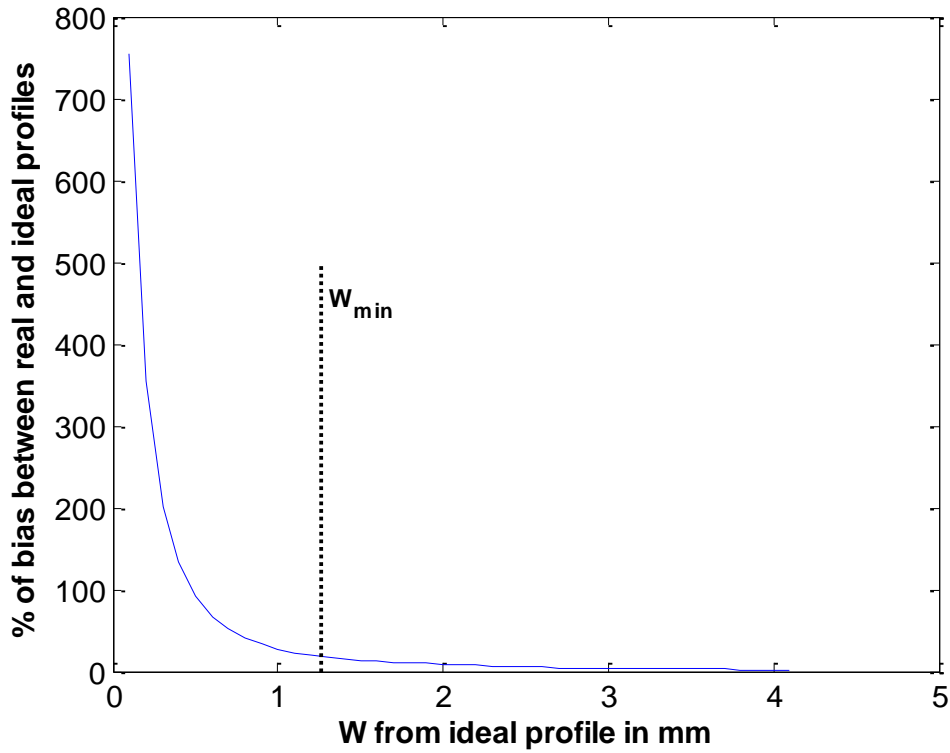
% Zoom on values higher than Wmin of previous plot
figure (22)
axes('FontSize',12)
plot (csimulades, errorc)
hold on
plot([MER MER],[0 500],'k:','Linewidth',1.5)
xlabel('W from ideal profile in mm','FontWeight','bold','FontSize',12)
ylabel('% of bias between real and ideal
profiles','FontWeight','bold',...
'FontSize',12)
axis([MER-0.5 cmaxacom/10 0 max(errorc(mer:end))+5])
text(MER+0.05,2, strcat('W_{min}'),'FontWeight','bold','FontSize',10)
%% IMAGES

```

%% Plot 1



%% Plot 2.1



%% Plot 2.2

