% First make an instance of the project class

problem = projectClass('DSPC monolayers');

% Define the parameters:

Parameters = {

% Name min val max fit?

{'Tails Thickness', 10, 20, 30, true};

{'Heads Thickness', 3, 11, 16, true};

{'Tails Roughness', 2, 5, 9, true};

{'Heads Roughness', 2, 5, 9, true};

{'Deuterated Tails SLD', 4e-6, 6e-6, 2e-5, true};

{'Hydrogenated Tails SLD', -0.6e-6, -0.4e-6, 0, true};

{'Deuterated Heads SLD', 1e-6, 3e-6, 8e-6, true};

{'Hydrogenated Heads SLD', 0.1e-6, 1.4e-6, 3e-6, true};

{'Heads Hydration', 0, 0.3, 0.5, true};

};

% Group these into layers:

H\_Heads = {'Hydrogenated Heads',...

'Heads Thickness',...

'Hydrogenated Heads SLD',...

'Heads Roughness',...

'Heads Hydration',...

'bulk out' };

D\_Heads = {'Deuterated Heads',...

'Heads Thickness',...

'Deuterated Heads SLD',...

'Heads Roughness',...

'Heads Hydration',...

'bulk out' };

D\_Tails = {'Deuterated Tails',...

'Tails Thickness',...

'Deuterated Tails SLD',...

'Tails Roughness'};%,...

%'Tails Hydration',...

%'bulk in'};

H\_Tails = {'Hydrogenated Tails',...

'Tails Thickness',...

'Hydrogenated Tails SLD',...

'Tails Roughness'};%,...

%'Tails Hydration',...

%'bulk in'};

% Add the parameters and Layers to the project:

problem.addParamGroup(Parameters);

problem.addLayerGroup({H\_Heads; D\_Heads; H\_Tails; D\_Tails});

% Increase the constr range for Substrate Roughness (param 1)

problem.setParamConstr(1,2,13);

% Need two backgrounds - one for D2O and for H2O

% Change the name of the first and add a new one for the second

% Also need a new backsPar

problem.setBacksParName(1,'Backs value ACMW');

problem.setBacksParValue(1,5.5e-6);

problem.addBacksPar('Backs Value D2O',1e-8,2.8e-6,1e-5);

problem.addBackground('Background D2O','constant','Backs Value D2O');

problem.setBackgroundValue(1,'name','Background ACMW');

problem.setBackgroundValue(1,3,'Backs Value ACMW');

% Also need an additional bulk out

problem.addBulkOut({'SLD ACMW' -1e-6,0.0,1e-6,true});

% Add the data files

d13ACM = dlmread('d13acmw20.dat');

d70d2O = dlmread('d70d2o20.dat');

problem.addData('H-tail / D-head / ACMW', d13ACM);

problem.addData('D-tail / H-head / D2O', d70d2O);

% Add the contrasts

problem.addContrast('name','D-tail/H-Head/D2O',...

'background','Background D2O',...

'resolution','Resolution 1',...

'scalefactor', 'Scalefactor 1',...

'nbs', 'SLD D2O',...

'nba', 'SLD air',...

'data', 'D-tail / H-head / D2O');

problem.setContrastModel(1,{'Deuterated tails','Hydrogenated heads'});

problem.addContrast('name','H-tail/D-Head/ACMW',...

'background','Background ACMW',...

'resolution','Resolution 1',...

'scalefactor', 'Scalefactor 1',...

'nbs', 'SLD ACMW',...

'nba', 'SLD air',...

'data', 'H-tail / D-head / ACMW');

problem.setContrastModel(2,{'hydrogenated tails','deuterated heads'});

% Set the fitting fitting flag on some parameters we need to fit

problem.setBacksPar(1,'fit',true);

problem.setBacksPar(2,'fit',true);

problem.setScalefactor(1,'fit',true);

problem.setBulkOut(1,'fit',true);

% Display problem

problem

% Make the controls class...

controls = controlsDef();

controls.parallel = 'points';

disp(controls)

[problem,results] = RAT(problem,controls);

disp(results)

figure(1); clf

plotRefSLD(problem,results)

controls.procedure = 'simplex'

[out,results] = RAT(problem,controls)

figure; clf

plotRefSLD(out,results)

save('twoContrastExample.mat','problem');