ORSO Lipid Example 1 - DSPC Bilayer Analysed Using a Standard Layers Model.

Start by making an empty instance of the project definition class:

```
problem = projectClass('Orso lipid example')
```

```
problem =
    experimentType: 'Standard Layers with (d,rho,rough) layers'
    experimentName: 'Orso lipid example'
          Geometry: 'air/substrate'

    Parameters: ------------------------------------------------------------------------------------------

    p            Name             Min    Value    Max    Fit?
    _    _____________________    ___    _____    ___    _____

    1    "Substrate Roughness"     1       3       5     true

    Layers: ----------------------------------------------------------------------------------------------

    Name    Thickness    SLD    Roughness    Hydration    Hydrate with
    ____    _________    ___    _________    _________    ____________

     0          0         0         0            0             0


    Bulk In: ---------------------------------------------------------------------------------------------

    p      Name       Min    Value    Max    Fit?
    _    _________    ___    _____    ___    _____

    1    "SLD Air"     0       0       0     false

    Bulk Out: --------------------------------------------------------------------------------------------

    p      Name         Min       Value       Max       Fit?
    _    _________    _______    ________    ________    _____

    1    "SLD D2O"    6.2e-06    6.35e-06    6.35e-06    false

    Scalefactors: ----------------------------------------------------------------------------------------

    p         Name          Min     Value    Max     Fit?
    _    _______________    ____    _____    ____    _____

    1    "Scalefactor 1"    0.02    0.23     0.25    false

    Backgrounds: -----------------------------------------------------------------------------------------

    (a) Background Parameters:
    p        Name          Min      Value     Max      Fit?
    _    _____________    _____    _____    _____    _____

    1    "Backs par 1"    1e-07    1e-06    1e-05    false

    (b) Backgrounds:
    p         Name            Type          Value 1       Value 2    Value 3    Value 4    Value 5
    _    _____________    __________    _____________    _______    _______    _______    _______
```

```
1    "Background 1"    "constant"    "Backs Par 1"      ""         ""         ""         ""

Resolutions: ------------------------------------------------------------------------------------------

(a) Resolutions Parameters:
p           Name            Min     Value    Max     Fit?
_    ____________________    ____    _____    ____    _____

1    "Resolution par 1"    0.01    0.03     0.05    false

(b) Resolutions:
p         Name             Type           Value 1           Value 2    Value 3    Value 4    Value 5
_    _____________    ___________    ___________________    _______    _______    _______    _______

1    "Resolution 1"    "gaussian"    "Resolution par 1"      ""         ""         ""         ""

Data: ------------------------------------------------------------------------------------------------

  Name         Data        Data Range       Simulation Range
________    __________    __________    ____________________

"Data 1"    "No Data"       "-"        "[ 0.0050 , 0.7000 ]"


Constrasts: ------------------------------------------------------------------------------------------

      p
_____________

"name"
"Data"
"Background"
"Bulk in"
"Bulk out"
"Scalefactor"
"Resolution"
"Model"
```

This is the standard class containing the model definition for any project. We add to it using the class methods, which are fairly self explanatory (although more detailed instructions are pending) -

```
methods(problem)
```

```
Methods for class projectClass:

addBackground       addLayer            getAllAllowedNames  setBackgroundValue  setBulkOut          setPar
addBacksPar         addLayerGroup       projectClass        setBacksPar         setContrast         setPar
addBulkIn           addParam            removeBacksPar      setBacksParConstr   setData             setPar
addBulkOut          addParamGroup       removeData          setBacksParName     setGeometry         setPar
addContrast         addQzshift          removeParam         setBacksParValue    setLayerValue       setPar
addData             addScalefactor      setBackgroundName   setBulkIn           setParamConstr      setSca

Methods of projectClass inherited from handle.
```

In this example, we will use a standard layers model. This defines layers in terms of thickness, SLD, roughness and hydration. These are then grouped into layers and the allocated to contrasts in the normal RasCAl way. For this sample, we have a DSPC bilayer on a Silicon substrate, which will be coated by an oxide layer. Ususally there is a hydration layer between the substrate and the lipid, although this depends on the exact conditions

of the measurement. Start by defining the parameters for the oxide layer. We need a thickness, SLD and hydration. The roughness is assumed to be the bulk substrate roughness.

```
Parameters = {
    %       Name                min         val         max     fit?
        {'Oxide thick',         10,         20,         25,     true   };
        {'Oxide SLD',           3e-6,       3.41e-6,    4e-6,   false  };
        {'Oxide Hydration'      0,          20,         30,     true   }};
```

Add these parameters to the project class, and group them into a layer to demonstrate how this is done:

```
    problem.addParamGroup(Parameters)
```

```
ans =
    experimentType: 'Standard Layers with (d,rho,rough) layers'
    experimentName: 'Orso lipid example'
          Geometry: 'air/substrate'

    Parameters: ------------------------------------------------------------------------------------------

    p            Name              Min      Value       Max      Fit?
    _    ____________________    ______    ________    ______    _____

    1    "Substrate Roughness"        1           3         5    true
    2    "Oxide thick"               10          20        25    true
    3    "Oxide SLD"              3e-06    3.41e-06    4e-06    false
    4    "Oxide Hydration"            0          20        30    true

    Layers: ----------------------------------------------------------------------------------------------

    Name    Thickness    SLD    Roughness    Hydration    Hydrate with
    ____    _________    ___    _________    _________    ____________

     0          0         0         0            0             0


    Bulk In: ---------------------------------------------------------------------------------------------

    p      Name       Min    Value    Max    Fit?
    _    _________    ___    _____    ___    _____

    1    "SLD Air"     0       0       0     false

    Bulk Out: --------------------------------------------------------------------------------------------

    p      Name         Min        Value        Max        Fit?
    _    _________    _______    ________    ________    _____

    1    "SLD D2O"    6.2e-06    6.35e-06    6.35e-06    false

    Scalefactors: ----------------------------------------------------------------------------------------

    p         Name           Min      Value     Max      Fit?
    _    _______________    _____    _____    _____    _____

    1    "Scalefactor 1"    0.02     0.23      0.25     false

    Backgrounds: -----------------------------------------------------------------------------------------

    (a) Background Parameters:
    p        Name          Min      Value      Max      Fit?
```

```
_    _____________    _____    _____    _____    _____

1    "Backs par 1"    1e-07    1e-06    1e-05    false

(b) Backgrounds:
p         Name             Type          Value 1       Value 2    Value 3    Value 4    Value 5
_    _____________    ___________    _____________    _______    _______    _______    _______

1    "Background 1"    "constant"    "Backs Par 1"      ""         ""         ""         ""

Resolutions: ------------------------------------------------------------------------------------

(a) Resolutions Parameters:
p           Name           Min      Value     Max      Fit?
_    ___________________    ____    _____    ____    _____

1    "Resolution par 1"    0.01    0.03     0.05    false

(b) Resolutions:
p         Name             Type           Value 1          Value 2    Value 3    Value 4    Value 5
_    _____________    ___________    ___________________    _______    _______    _______    _______

1    "Resolution 1"    "gaussian"    "Resolution par 1"      ""         ""         ""         ""

Data: --------------------------------------------------------------------------------------------

  Name         Data         Data Range       Simulation Range
________    _________    ___________    ____________________

"Data 1"    "No Data"       "-"         "[ 0.0050 , 0.7000 ]"


Constrasts: --------------------------------------------------------------------------------------

      p
_____________

"name"
"Data"
"Background"
"Bulk in"
"Bulk out"
"Scalefactor"
"Resolution"
"Model"
```

```
% Now make the oxide layer
Oxide =     {'Oxide Layer',...          % Name of the layer
             'Oxide thick',...          % Layer thickness
             'Oxide SLD',...            % Layer SLD
             'Substrate Roughness',...  % Layer roughness
             'Oxide Hydration',...      % Oxide hydration (precent)
             'bulk out' };              % Which bulk phase is hydrating the layer

% Add this to the project...
problem.addLayer(Oxide)
```

```
ans =
    experimentType: 'Standard Layers with (d,rho,rough) layers'
    experimentName: 'Orso lipid example'
          Geometry: 'air/substrate'

    Parameters: --------------------------------------------------------------------------------------
```

p	Name	Min	Value	Max	Fit?
1	"Substrate Roughness"	1	3	5	true
2	"Oxide thick"	10	20	25	true
3	"Oxide SLD"	3e-06	3.41e-06	4e-06	false
4	"Oxide Hydration"	0	20	30	true

Layers:

p	Name	Thickness	SLD	Roughness	Hydration	Hy
1	"Oxide Layer"	"Oxide thick"	"Oxide SLD"	"Substrate Roughness"	"Oxide Hydration"	"

Bulk In:

p	Name	Min	Value	Max	Fit?
1	"SLD Air"	0	0	0	false

Bulk Out:

p	Name	Min	Value	Max	Fit?
1	"SLD D2O"	6.2e-06	6.35e-06	6.35e-06	false

Scalefactors:

p	Name	Min	Value	Max	Fit?
1	"Scalefactor 1"	0.02	0.23	0.25	false

Backgrounds:

(a) Background Parameters:

p	Name	Min	Value	Max	Fit?
1	"Backs par 1"	1e-07	1e-06	1e-05	false

(b) Backgrounds:

p	Name	Type	Value 1	Value 2	Value 3	Value 4	Value 5
1	"Background 1"	"constant"	"Backs Par 1"	""	""	""	""

Resolutions:

(a) Resolutions Parameters:

p	Name	Min	Value	Max	Fit?
1	"Resolution par 1"	0.01	0.03	0.05	false

(b) Resolutions:

p	Name	Type	Value 1	Value 2	Value 3	Value 4	Value 5
1	"Resolution 1"	"gaussian"	"Resolution par 1"	""	""	""	""

```
Data: ------------------------------------------------------------------------------------------

  Name        Data       Data Range      Simulation Range
________    _________    __________    ____________________

"Data 1"    "No Data"       "-"        "[ 0.0050 , 0.7000 ]"


Constrasts: ------------------------------------------------------------------------------------

      p
_____________

"name"
"Data"
"Background"
"Bulk in"
"Bulk out"
"Scalefactor"
"Resolution"
"Model"
```

Now we'll build the layers for the lipid, The bilayer is symmetrical, so we can have mostly the same values for the inner and outer tails and heads. We have to be a bit careful with roughness' however, since we want to have a slightly different roughness for the head/water interface and the head/alkyl interface, and for layer model in this geometry the roughnes for each layer refers to the next interface. So we'll make separate layers for inner and outer lipids, but all sharing the same parameters, and just differeing in the roughness order.

Define the parameters we will need:

```
% Bilayer parameters:
bilParams = {
        {'Bilayer head thick',  5,          10,         15,     true    };
        {'Bilayer head sld',    1e-6,       1.47e-6,    1.6e-6, true    };
        {'Bilayer heads hydr',  20,         30,         40,     true    };
        {'Bilayer Heads rough'  5,          7,          15,     true    };
        {'Bilayer tails thick', 10,         15,         20,     true    };
        {'Bilayer tails SLD',   -5e07,      -4e-7,      -1e-7,  false   };
        {'Bilayer tails hydr',  0,          10,         20,     true    };
        {'Bilayer tails rough', 5,          9,          15,     true    };
};

% We want the water layer to be matched in SLD to the bulk water phase. So
% we give it an SLD of 0, and a hydration of 100%, and make these
% non-fittable

watParams = {
        {'Water thick',         5,          1,          15,     true    };
        {'Water SLD',           0,          0,          0,      false   };


}
```