User Documentation

ChroMo

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# Input Data

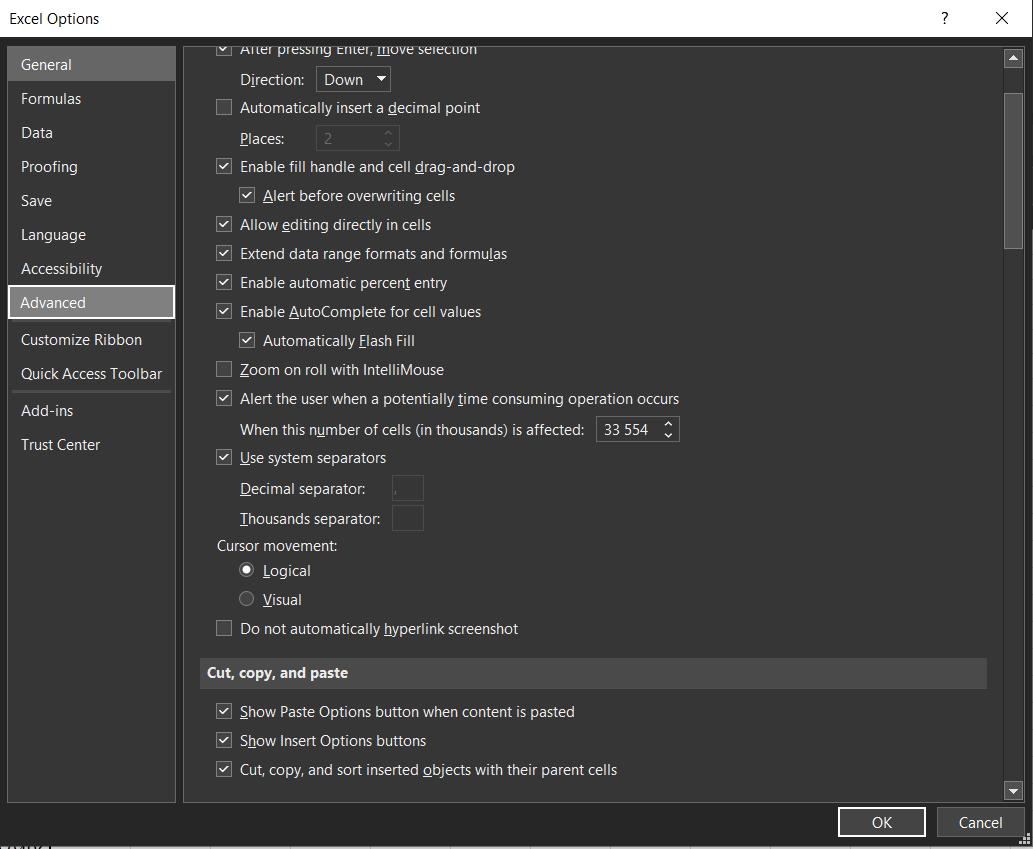
Input data needs to be in one folder which contains any amount of .xlsx files.

## Excel File

MS Excel files (.xlsx) needs to be in the form of template contained in the program folder.

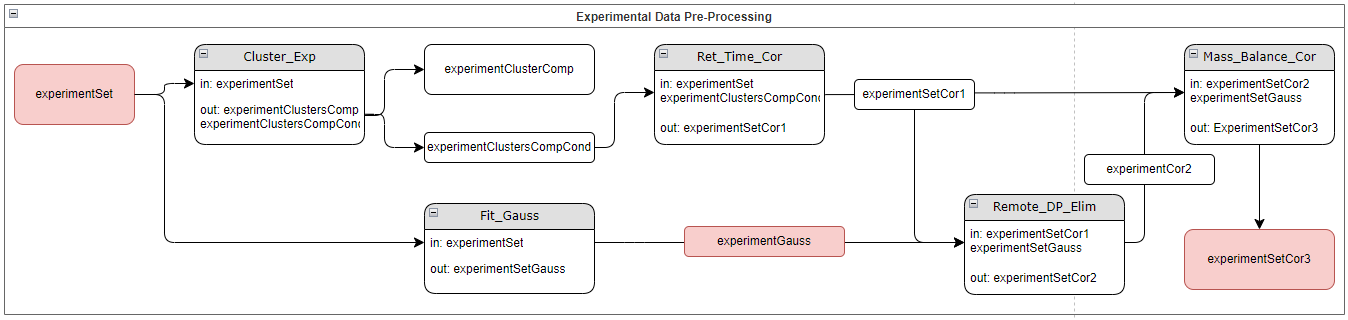
### Excel Settings Requirements

Thousand separator needs to be set as empty input. Otherwise, it can cause problems with values reading.



# Program Execution

## Data pre-processing

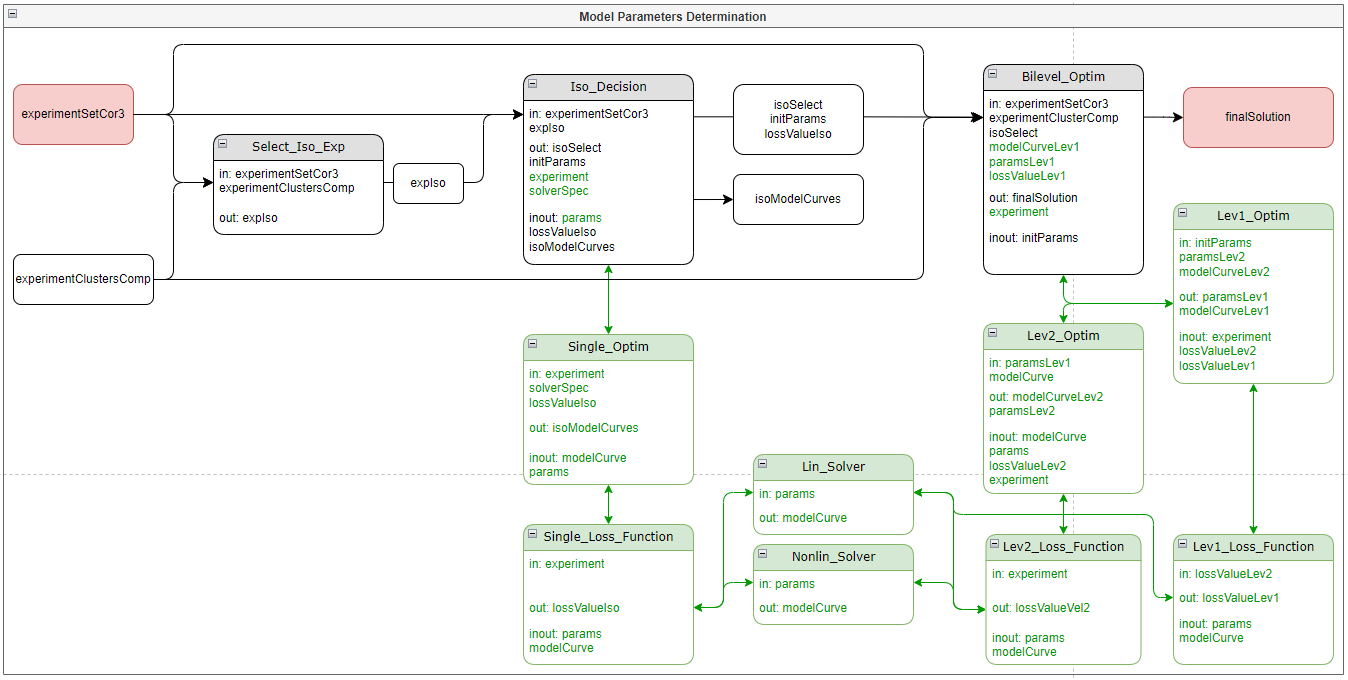


runtime question to user: Use fitted Gauss curve directly as a corrected datapoints? Y/N

if Y, then we skip Remote\_DP\_Elim.py and use the output of Fit\_Gauss.py directly as an input to Mass\_Balance\_Cor.py

if N, then we stick to our original plan (use Gaussian just for elimination of remote points base on threshold)

## Model fitting



# Results

# Functions and Objects Documentation

## Objects

### ExperimentSet

*class objects.ExperimentSet*

#### Description

Class representing group of experiments

#### Attributes

*experiments(list[Experiment])* - List of Experiment objects

*metadata(Metadata)* - Information about experiment set

### Experiment

*class objects.Experiment*

#### Description

Class representing experiment

#### Attributes

*experimentCondition(ExperimentCondition)* - Conditions of the experiment

*experimentComponents(list[ExperimentComponent])* - Components of the experiment

*metadata(Metadata)* - Information about experiment

### ExperimentCondition

*class objects.ExperimentCondition*

#### Description

Class representing conditions of an experiment

#### Attributes

*columnDiameter(float)* - Diameter of column used in experiment

*columnLength(float)* - Length of column used in experiment

*feedVolume(float)* - Volume of feed in experiment

*feedTime(float)* - Time of feed in experiment

*flowRate(float)* - low rate in experiment

### ExperimentComponent

*class objects.ExperimentComponent*

#### Description

Class representing component in an experiment

#### Attributes

*concentrationTime(pandas.DataFrame)* - Table of times and concentrations measured in experiment

*feedConcentration(float)* - Concentration of component in feed

*name(str)* - Name of the component

*experiment(Experiment)* - Reference to experiment with this component

### ExperimentClusters

*class objects.ExperimentClusters*

#### Description

Class representing clusters of components from multiple experiments

#### Attributes

*clusters(dict[str:list[ExperimentComponents]])* - Dictionary of component clusters

*metadata(Metadata)* - Information about clusters

### Metadata

*class objects.Metadata*

#### Description

Class representing information about other objects

#### Attributes

*date(str)* - Relevant date

*description(str)* - Description of the object

*path(str)* - Path to the source experiment(s)

### Operator

*class objects.Operator*

#### Description

Class managing the workflow of the program and comunication with the user

#### Methods

##### Start

*method objects.Operator.Start()*

###### Description

Starts and manages the workflow

##### Setting\_Parameters

*method objects.Operator.Setting\_Parameters()*

###### Description

Asks user to input relevant parameters

###### Returns

List of parameters(*list[float]*)

##### Load\_Experiment\_Set

*method objects.Operator.Load\_Experiment\_Set(path)*

###### Description

Creates an ExperimentSet object from excel files

###### Parameters

*path(str)* - Path to the files

###### Returns

ExperimentSet object(*ExperimentSet*)

##### Cluster\_By\_Component

*method objects.Operator.Cluster\_By\_Component(experimentSet)*

###### Description

Creates a ExperimentClusters object based on component

###### Parameters

*experimentSet(ExperimentSet)* - Experiment set to cluster

###### Returns

ExperimentClusters object(*ExperimentClusters*)

##### Cluster\_By\_Condition

*method objects.Operator.Cluster\_By\_Condition(experimentSet)*

###### Description

Creates a ExperimentClusters object based on component and condition of the experiment

###### Parameters

*experimentSet(ExperimentSet)* - Experiment set to cluster

###### Returns

ExperimentClusters object(*ExperimentClusters*)

##### Cluster\_By\_Condition2

*method objects.Operator.Cluster\_By\_Condition2(experimentSet)*

###### Description

Similar as Cluster\_By\_Condition, different cluster implementation

###### Parameters

*experimentSet(ExperimentSet)* - Experiment set to cluster

###### Returns

ExperimentClusters object(*ExperimentClusters*)

##### Cluster\_Match

*method objects.Operator.Cluster\_Match(comp1, comp2, tolerance = 0.05)*

###### Description

Method helping clustering methods to decide if two components are similar enough

###### Parameters

*comp1(ExperimentComponent)* - First component for comparison

*comp2(ExperimentComponent)* - Second component for comparison

*tolerance(float)* - Relative tolerance for similarity decision

###### Returns

Whether the two components are similar(*bool*)

##### Create\_Key

*method objects.Operator.Create\_Key(comp)*

###### Description

Method helping clustering methods to create key for dictionary

###### Parameters

*comp(ExperimentComponent)* - Component from which the key is created from

###### Returns

Key for clusters dictionary(*str*)

## Analysis and Debugging functions

### Compare\_ExperimentSets

*function functions.Compare\_ExperimentSets(experimentSet1, experimentSet2)*

#### Description

Compares two experiment sets and allows user to find differences.

#### Parameters

*experimentSet1(ExperimentSet)* - First experiment set to compare.

*experimentSet2(ExperimentSet)* - Second experiment set to compare.

### Loss\_Function\_Analysis

*function functions.Loss\_Function\_Analysis(experimentClusterComp, component='Sac', xstart = 0, ystart = 0, xend = 5002, yend = 5002, xstep = 50, ystep = 50, porosityStart = 0.2, porosotyEnd = 1, porosityStep = 0.1)*

#### Description

Allows user to analyze results of Lev2\_Loss\_Function with specified input values.

#### Parameters

*experimentClusterComp(ExperimentCluster)* Cluster of components to analyze.

*component(str)* - Specified name of component to analyze.

*xstart(int)* - Start of interval of Henry constant values for analysis.

*ystart(int)* - Start of interval of Dispersion coeficient values for analysis.

*xend(int)* - End of interval of Henry constant values for analysis.

*yend(int)* - End of interval of Dispersion coeficient values for analysis.

*xstep(int)* - Step of Henry constant values from interval for analysis.

*ystep(int)* - Step of Dispersion coeficient values from interval for analysis.

*porositystart(float)* - Start of interval of porosity values for analysis.

*porosityend(float)* - End of interval of porosity values for analysis.

*porositystep(float)* - Step of porosity values from interval for analysis.