# PAE Model Bank – User Guide

The application provides saved models within itself which the user can select for further exploration

It contains 5 functionalities that is Model Introduction, Model and Data Import, Visualization, Simulation and Optimisation

Model Introduction: Provides the name of the model along with its owner and information about the model selected

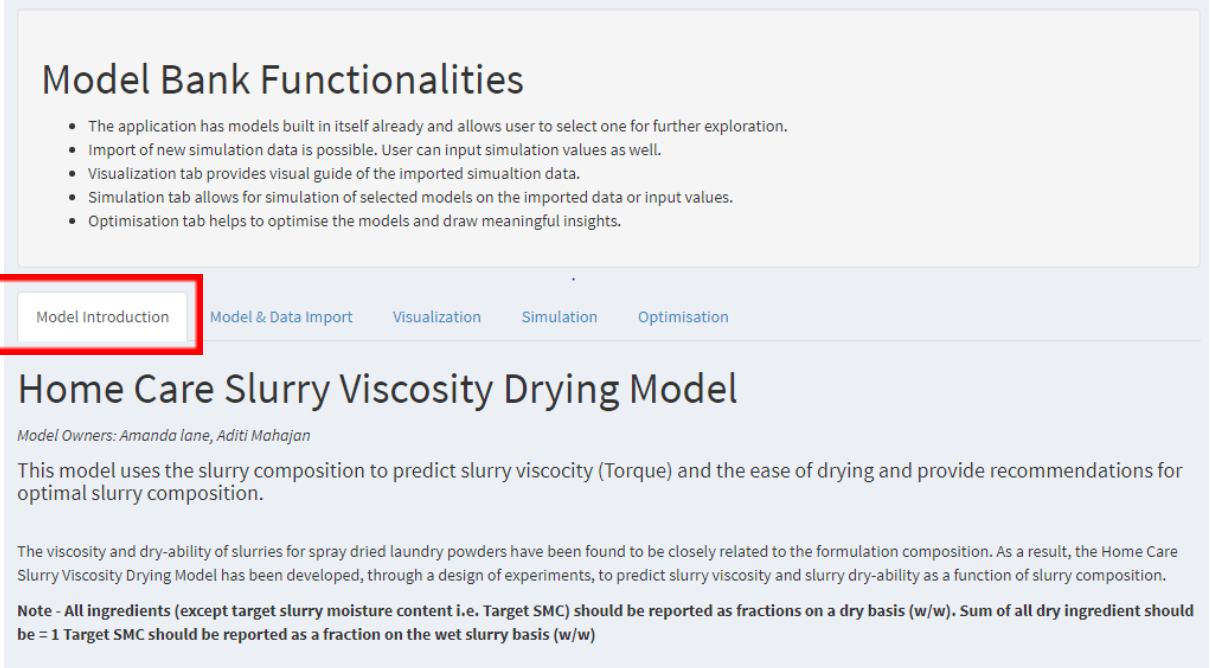
Model and Data Import: Enables user to see the equations that are saved within a given model and allows user to manually simulate a model or import a dataset to view the results of simulation.

Visualization: Provides univariate, Bivariate and Multivariate analysis of the dataset that is imported

Simulation: This tab is split into two manual entry and import data simulation respectively. The manual entry simulation reflects outcome of the input values for simulation in the Model and data import page whereas the Import data simulation shows the predictions based on the dataset that is previously imported.

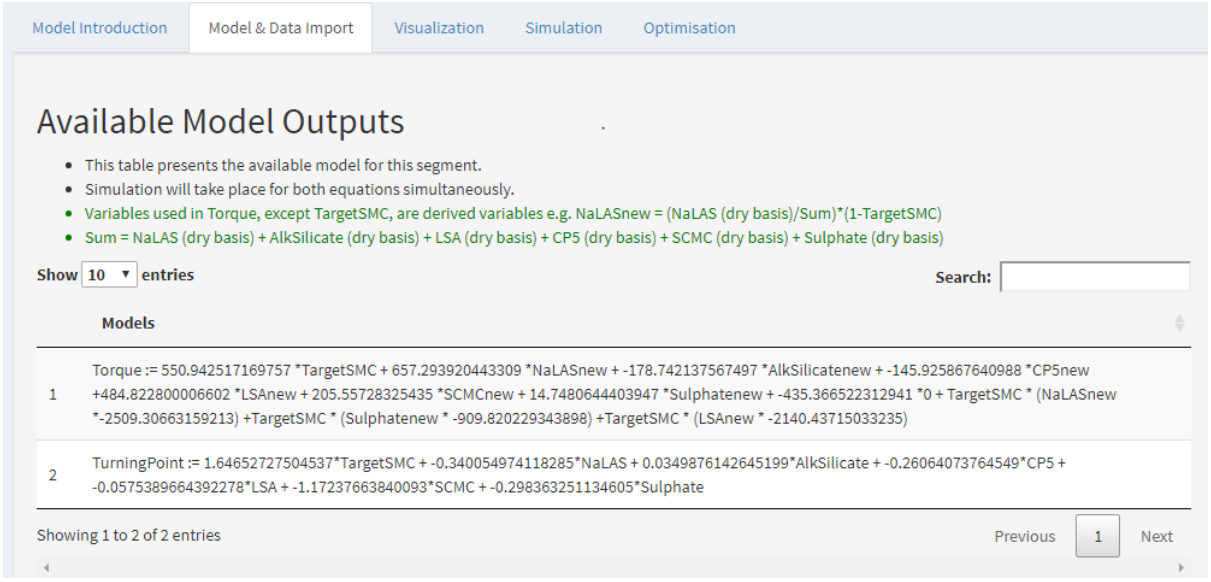
Optimisation: This tab enables user to optimize the selected equation based on constraints defined and the lower and upper limits of the predictor variables.

## 1- Model Introduction




- Model introduction provides the information about the model along with its owner.

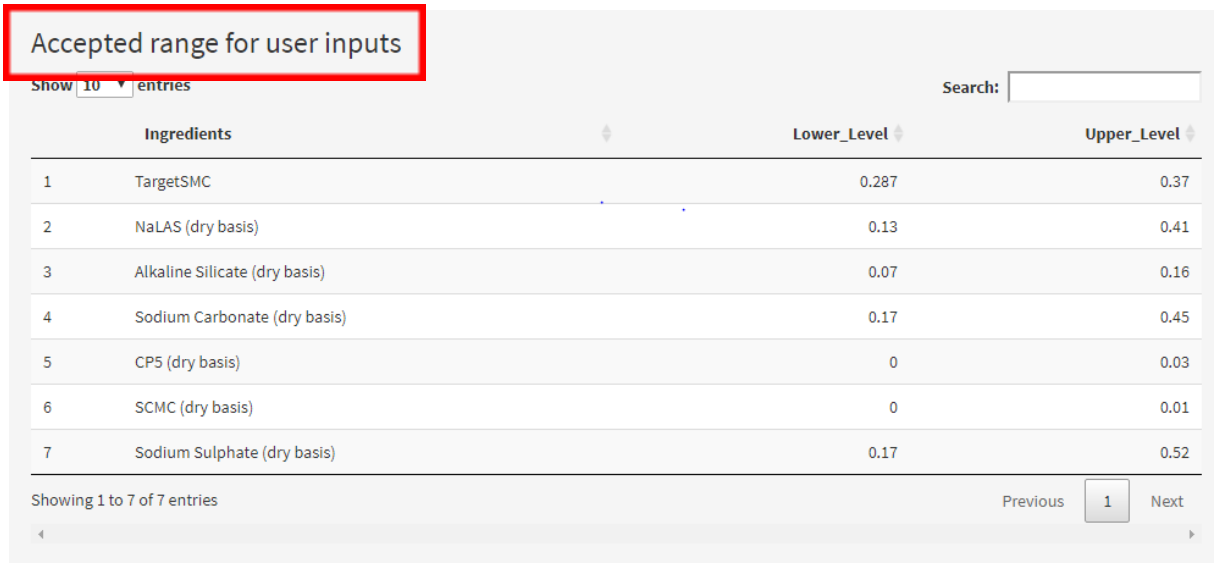
## 2 -Model and Data Import:



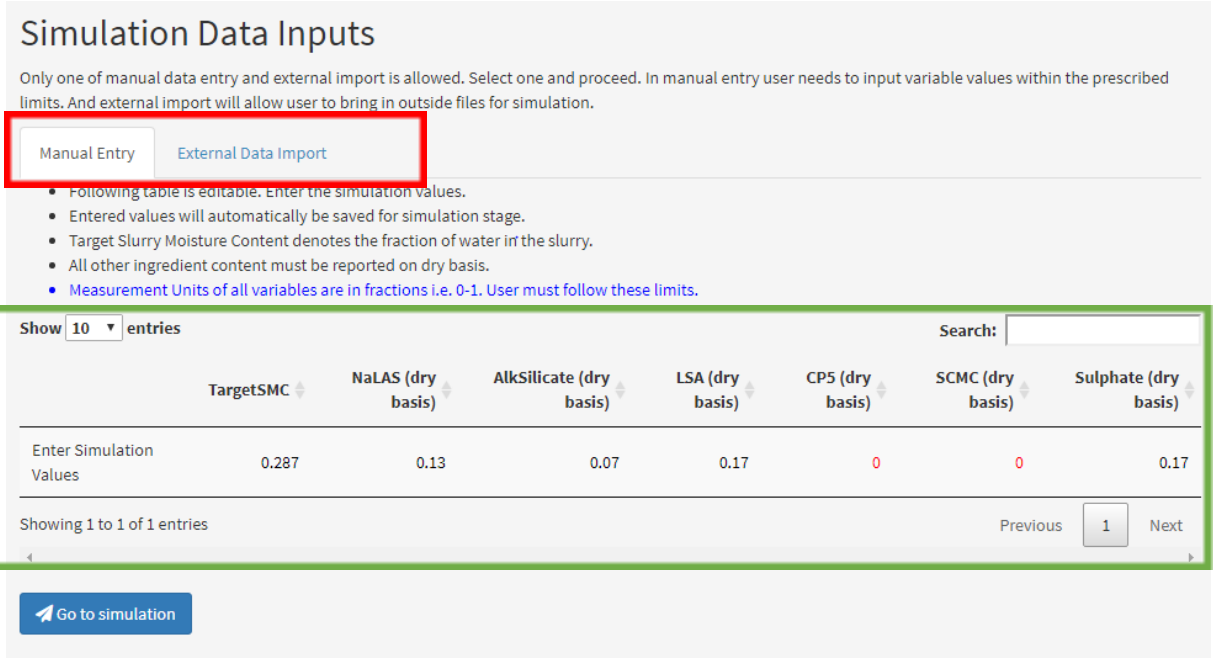

- Available model Outputs show the equations that are provided within the models.

### Manual Entry Simulation:

Within Simulation Data Inputs the user can pick manual entry simulation of external data import.

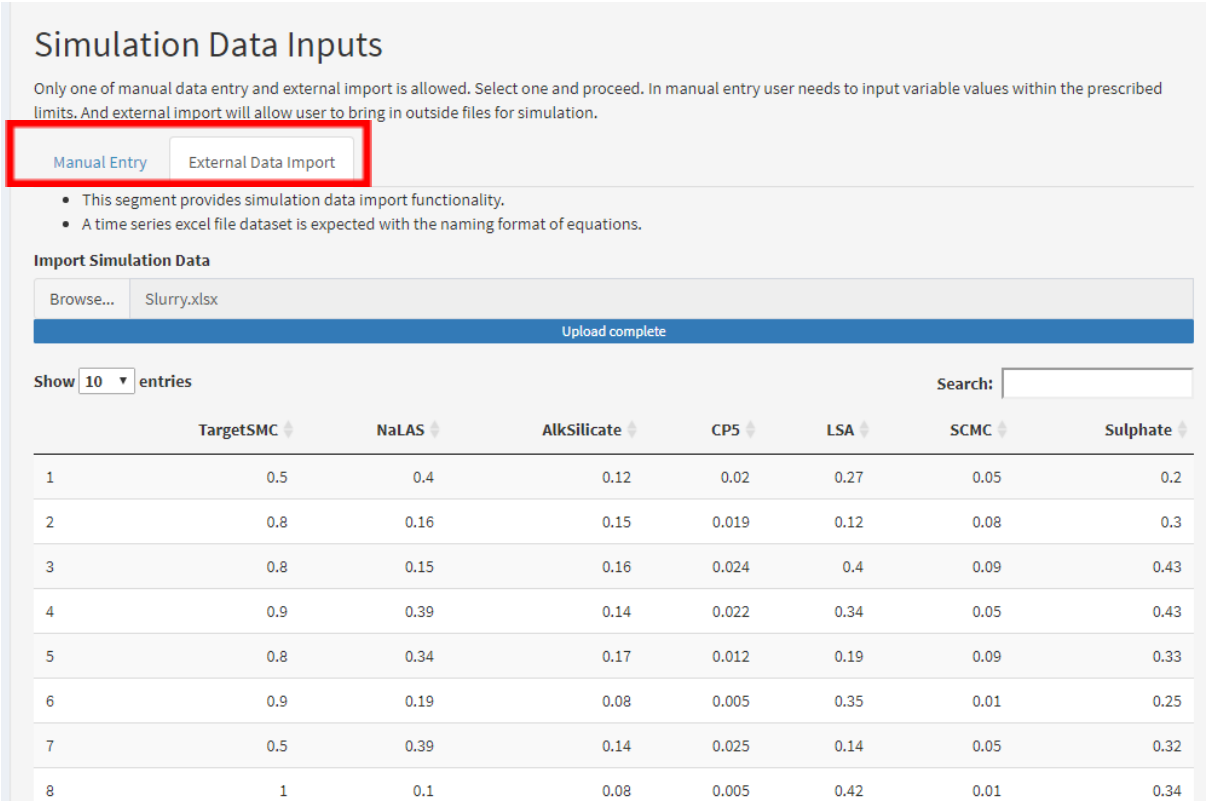



- The above table shows the lower and upper limits for all the predictors




- The red box shows that the selection is manual entry simulation
- This sub division enables the user to manually input various values of the predictor variables to see its corresponding response variable.
- The table in green is the input table where the values for various predictors need to be given by the user.
- If the predictor value falls outside the range, it will turn red.
- The user can move to the simulation page by clicking on the “Go to Simulation” button.

## External Data Import



Simulation Data Inputs

Only one of manual data entry and external import is allowed. Select one and proceed. In manual entry user needs to input variable values within the prescribed limits. And external import will allow user to bring in outside files for simulation.

Manual Entry | External Data Import

- This segment provides simulation data import functionality.
- A time series excel file dataset is expected with the naming format of equations.

**Import Simulation Data**

Browse... Slurry.xlsx

Upload complete

Show 10 entries Search:

| | TargetSMC | NaLAS | AlkSilicate | CP5 | LSA | SCMC | Sulphate |
|---|---|---|---|---|---|---|---|
| 1 | 0.5 | 0.4 | 0.12 | 0.02 | 0.27 | 0.05 | 0.2 |
| 2 | 0.8 | 0.16 | 0.15 | 0.019 | 0.12 | 0.08 | 0.3 |
| 3 | 0.8 | 0.15 | 0.16 | 0.024 | 0.4 | 0.09 | 0.43 |
| 4 | 0.9 | 0.39 | 0.14 | 0.022 | 0.34 | 0.05 | 0.43 |
| 5 | 0.8 | 0.34 | 0.17 | 0.012 | 0.19 | 0.09 | 0.33 |
| 6 | 0.9 | 0.19 | 0.08 | 0.005 | 0.35 | 0.01 | 0.25 |
| 7 | 0.5 | 0.39 | 0.14 | 0.025 | 0.14 | 0.05 | 0.32 |
| 8 | 1 | 0.1 | 0.08 | 0.005 | 0.42 | 0.01 | 0.34 |

- The red box shows that the selection is External data simulation
- Once the dataset is successfully uploaded, we see the complete blue line complete and also the dataset imported is shown below.
- If there is a predictor missing in the dataset imported the app will show a pop up but will continue to simulate assuming the value of that predictor as 0.

## 2- Visualization

| | TargetSMC | NaLAS | AlkSilicate | CP5 | LSA | SCMC | Sulphate |
|---|---|---|---|---|---|---|---|
| 1 | 0.5 | 0.4 | 0.12 | 0.02 | 0.27 | 0.05 | 0.2 |
| 2 | 0.8 | 0.16 | 0.15 | 0.019 | 0.12 | 0.08 | 0.3 |
| 3 | 0.8 | 0.15 | 0.16 | 0.024 | 0.4 | 0.09 | 0.43 |
| 4 | 0.9 | 0.39 | 0.14 | 0.022 | 0.34 | 0.05 | 0.43 |
| 5 | 0.8 | 0.34 | 0.17 | 0.012 | 0.19 | 0.09 | 0.33 |
| 6 | 0.9 | 0.19 | 0.08 | 0.005 | 0.35 | 0.01 | 0.25 |
| 7 | 0.5 | 0.39 | 0.14 | 0.025 | 0.14 | 0.05 | 0.32 |
| 8 | 1 | 0.1 | 0.08 | 0.005 | 0.42 | 0.01 | 0.34 |
| 9 | 0.2 | 0.21 | 0.08 | 0.019 | 0.29 | 0.02 | 0.14 |
| 10 | 0.6 | 0.18 | 0.13 | 0.019 | 0.23 | 0.1 | 0.46 |

Showing 1 to 10 of 50 entries Previous 1 2 3 4 5 Next

Go to Visualization

- Once the dataset is imported, click on “Go to Visualization” to further explore the dataset.

Model Introduction | Model & Data Import | Visualization | Simulation | Optimisation

Visual guide for imported data.

- This tab presents visualizations of the externally imported data.
- First two graphs allow overlapping of two variables on Y axis.
- While the first graph presents linear trend through line graph, the second graph presents linear regression based trend in data.
- Finally a histogram is presented.

### Scatter Plot

**X axis**

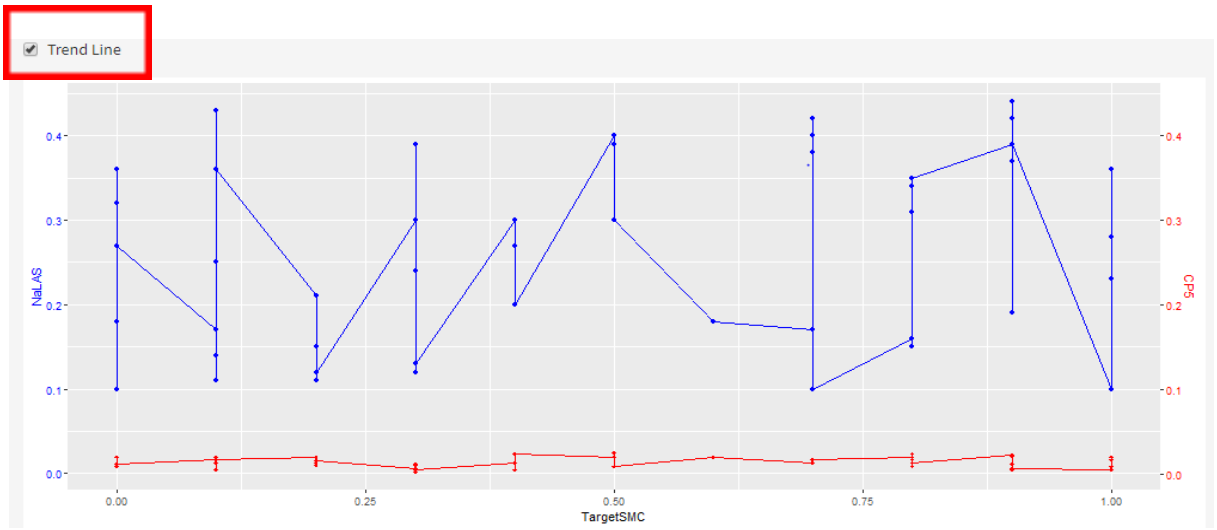
TargetSMC

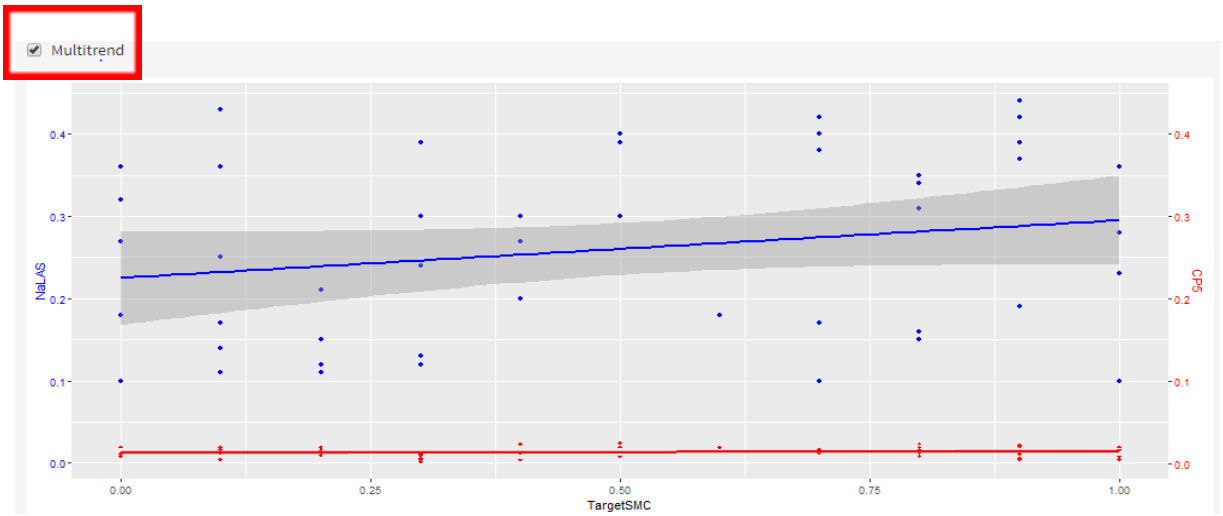
**Y axis**

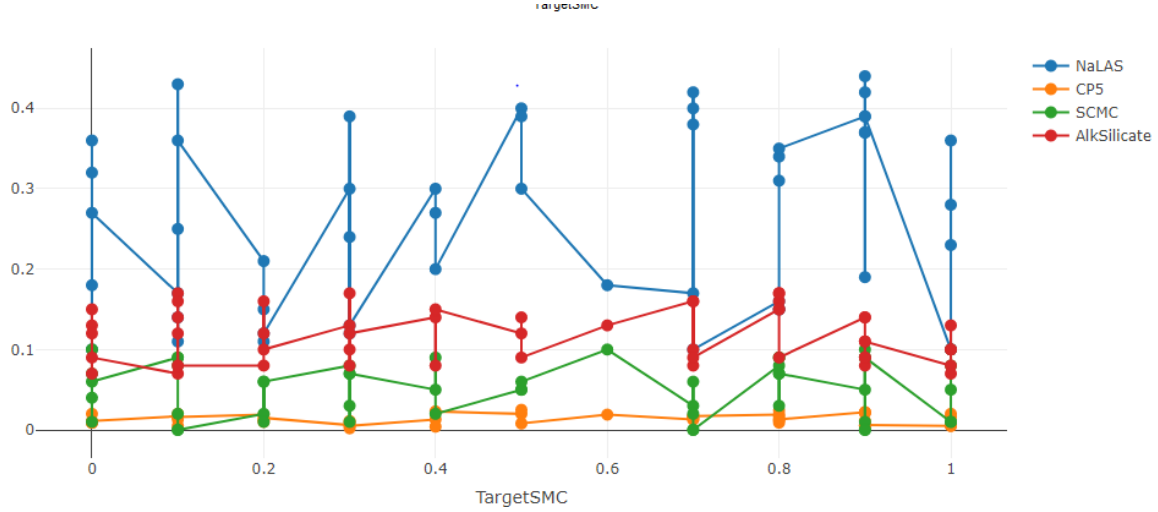
NaLAS

- First two graphs allow for double Y axis selection with single x axis.
- It takes the first two selections of y-axis for plotting. Linear regression method is used for creating trendlines in second graph.
- Checkboxes can be used for adding or removing the trends in graph.

- The above page appears after clicking the button.
- Select the desired X and Y variables from the drop down.
- Only 1 variable selection is allowed for X axis, whereas up to 4 can be selected for Y axis

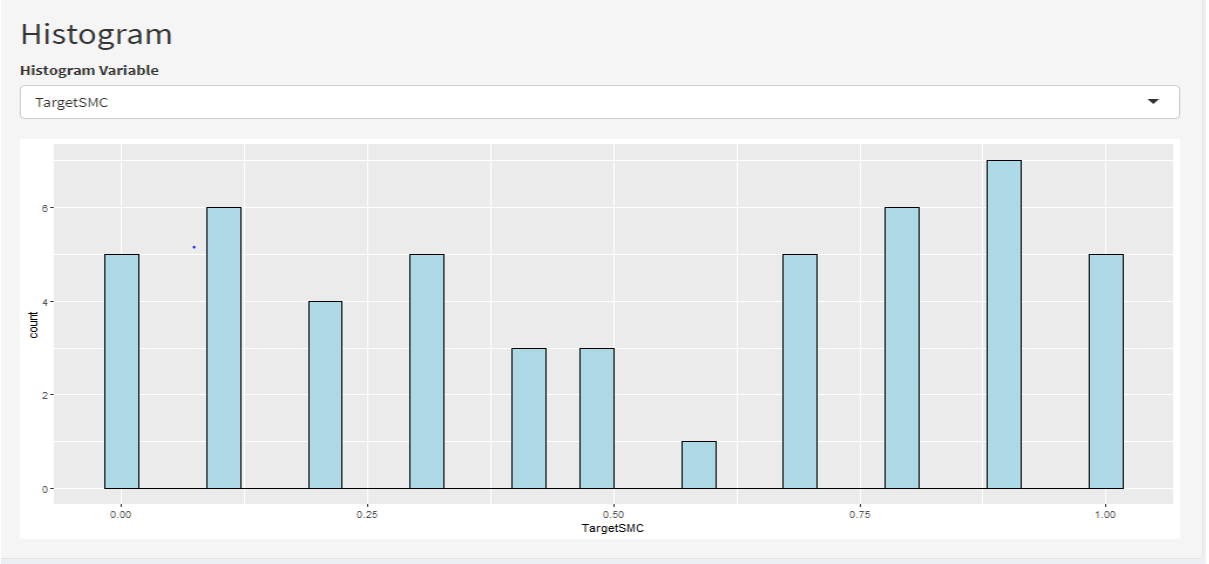



- The first two graphs allow for double Y axis selection with single X axis selection.

- It takes the first two selection of the Y axis to plot linear regression of X against the respective Y
- Check boxes for trendline and multitrend lines can be selected or unselected to view the trendline based on preference.
- The third graph is a scatter plot along with the trendline of all four variables selected for the Y axis.
- The histogram at the end provides distribution of each variable which can be selected through the drop down

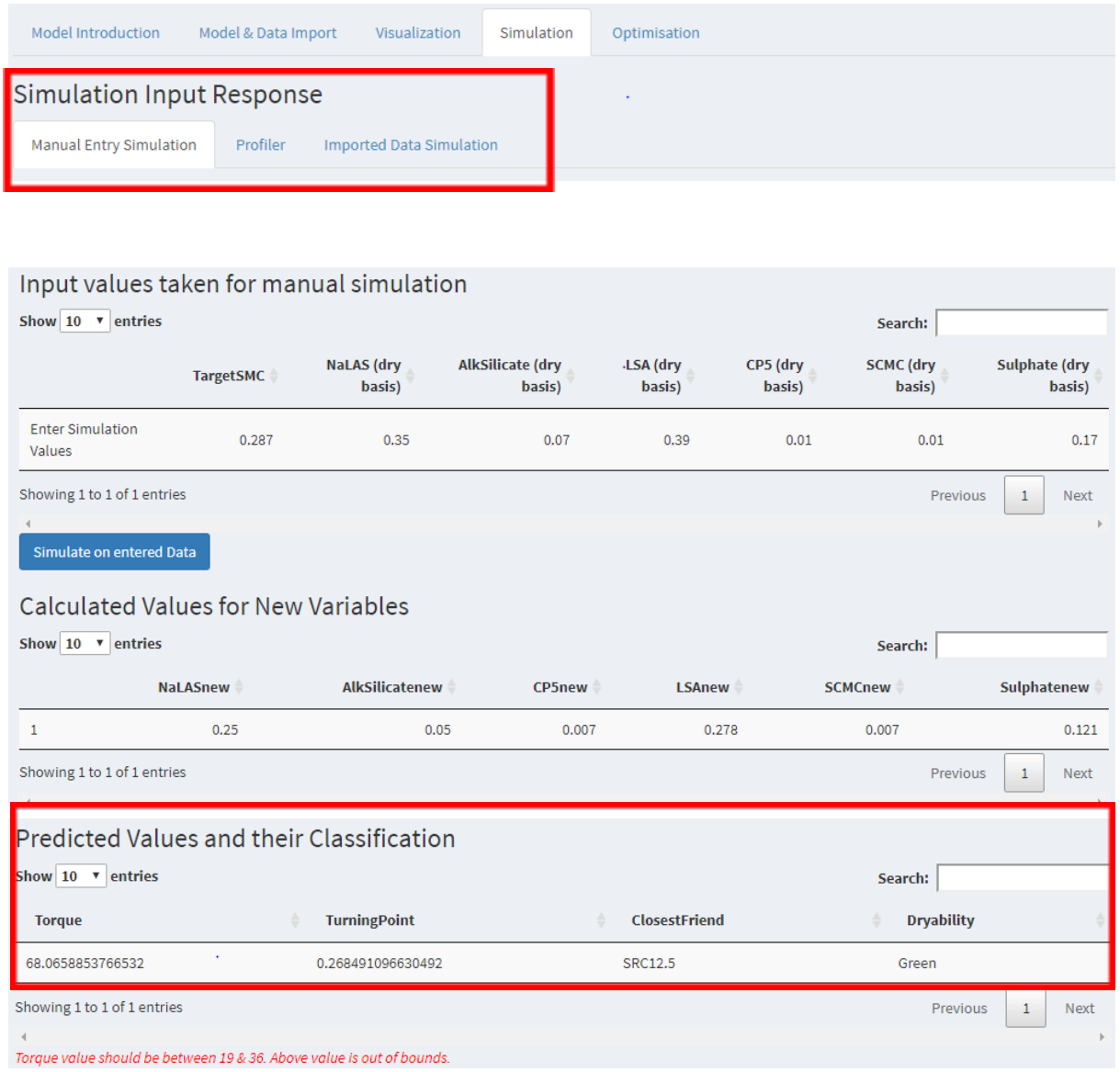


## 3- Simulation

The simulation page is split into 3 parts, Manual entry simulation, Profiler and Export data simulation

### Manual Entry Simulation

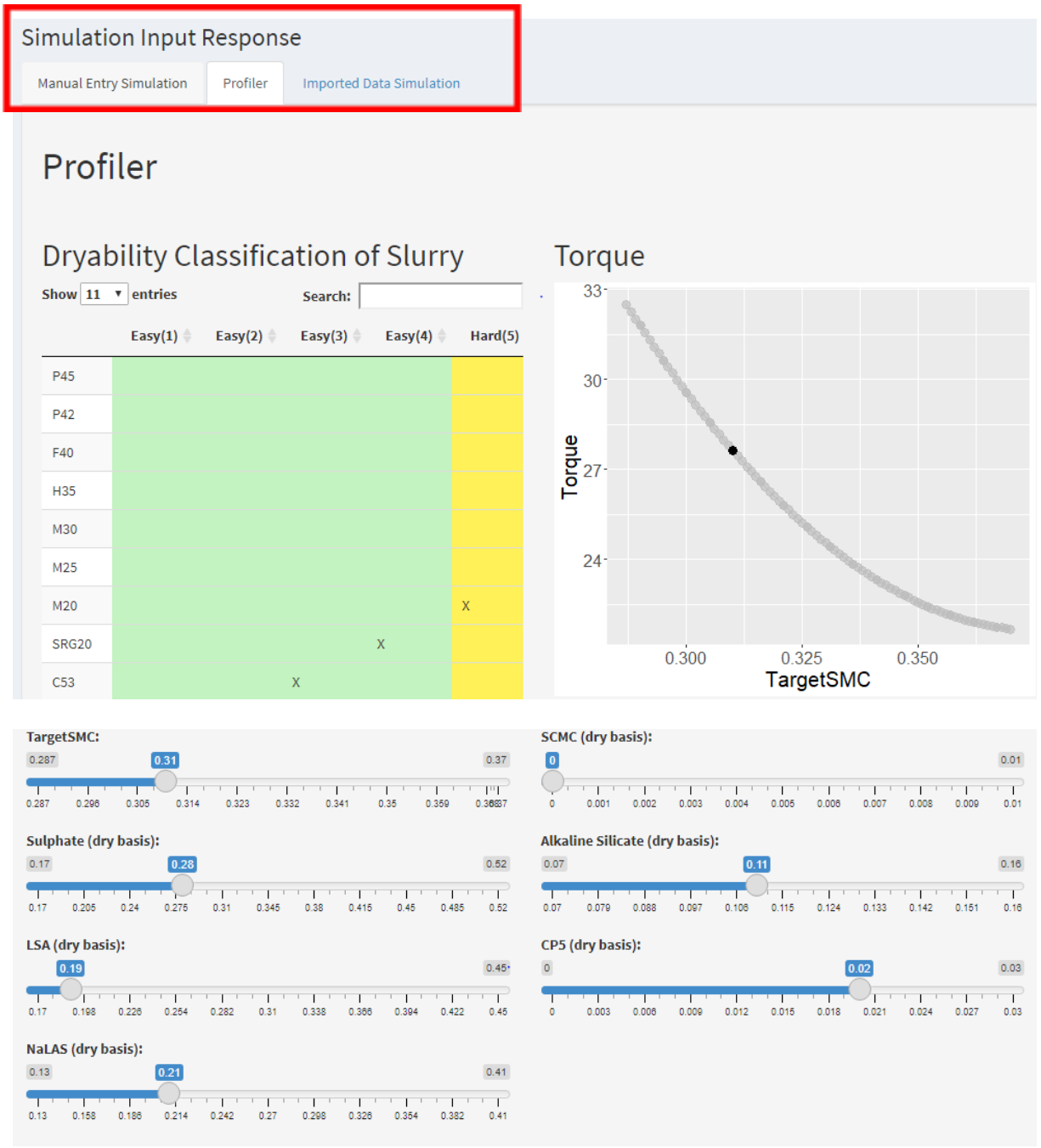
Manual Entry simulation provides capability of simulating on input values (Provided and model and Data import Page)




- The red box shows the selection of manual entry simulation
- The table “Input values taken for Manual Simulation” acts as a check to reconfirm the values of various predictors.
- Once the values are checked, click on “Simulation on entered data”
- The “Calculated Values for New Variables” show all the new values that are calculated based on the given predictor values.
- The final table “Predicted values and their classification”/ “Predicted Values” show the results generated for the following inputs.

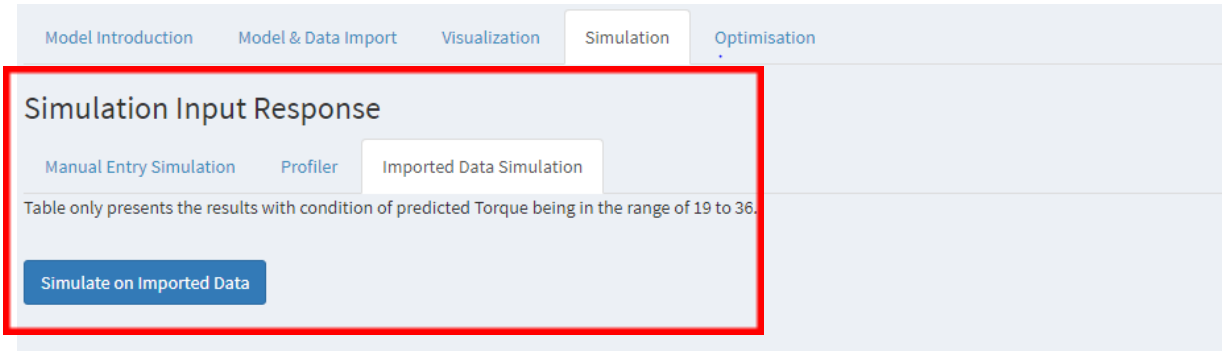

- The graph shows where the value of turning point lies with the tick mark and shows its Closest friend and Dryability
- “Download above results” saved the input values taken for manual simulation along with its output.
-

## Profiler



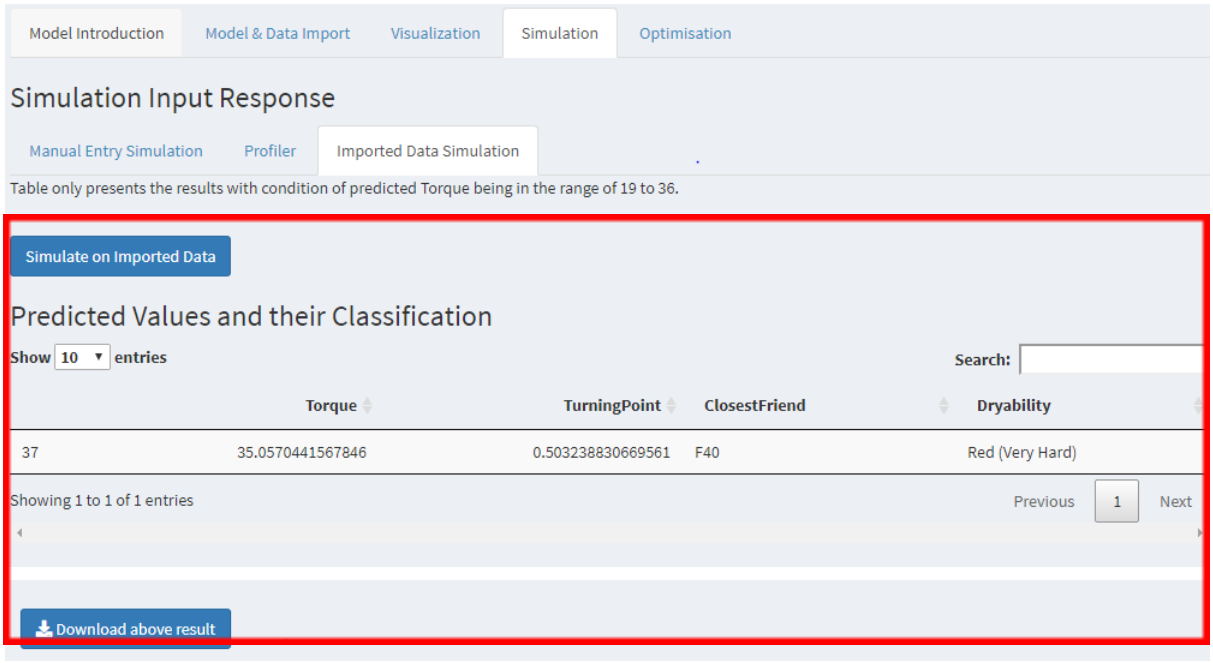

- The red box shows the selection as profiler
- The profiler allows user to scroll for various values of the predictors
- The graphs on top change as per the input changes in the scroller based for various response variable. Changes in response variables through changing sliderinput except the x axis variable is reflected through change in y axis range.

## Import data simulation




- After the dataset is imported in Model & Data Import Page
- Click on "Simulate on Imported Data" to see the values of response variables based on the dataset imported
- The red box shows the selection of import data simulation and the simulate button.

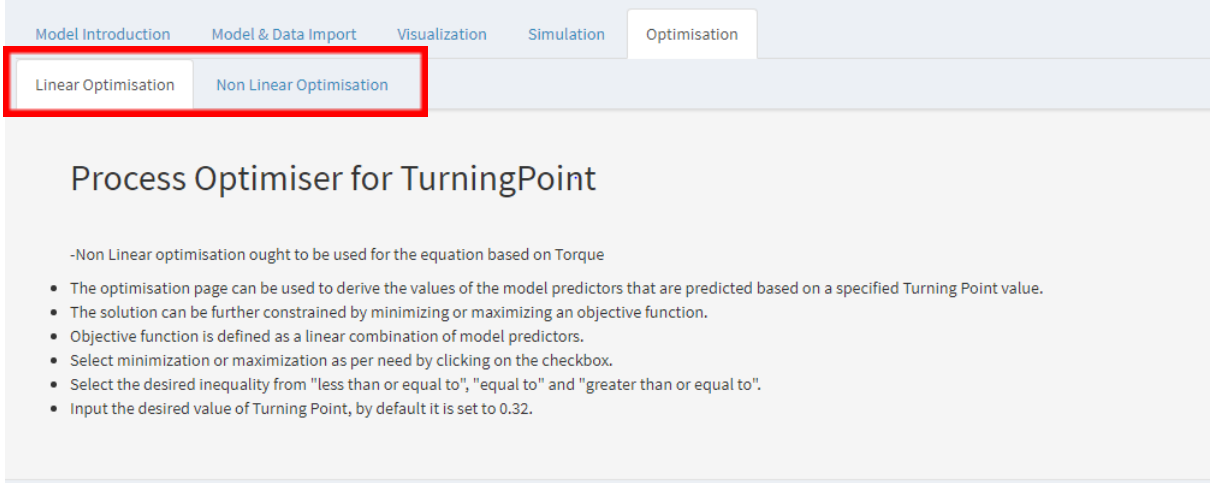
Once the button is pressed the results will be shown as following




- "Download Above Results" saved the outcome of import data simulation

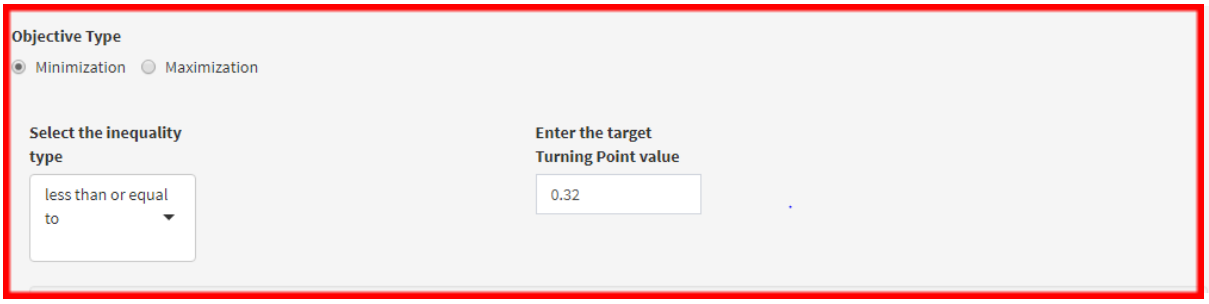
## 4- Optimisation

The optimisation page can be used to derive values for model predictors that are predicted based on a specified target variable.

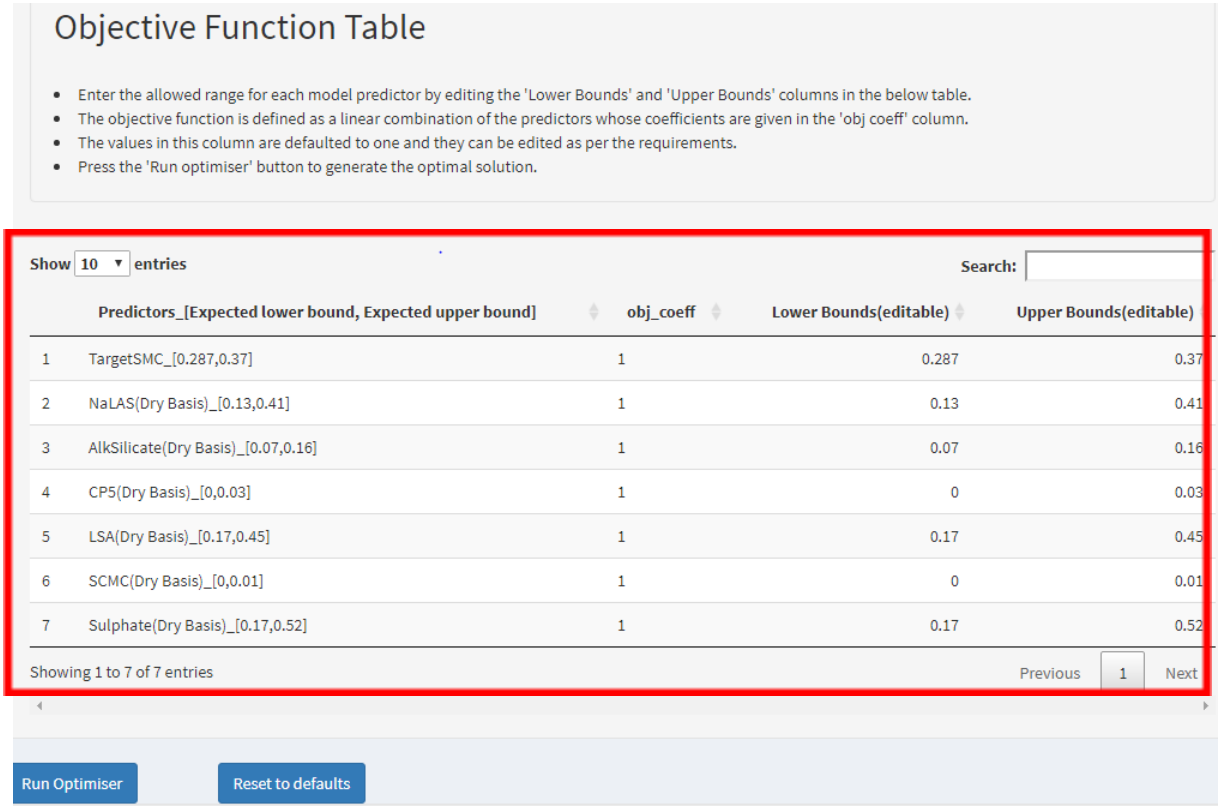



- The optimisation page shows linear and non-linear optimisation
- The red box shows the selection as linear optimisation
- All the linear equations within the model are optimised here

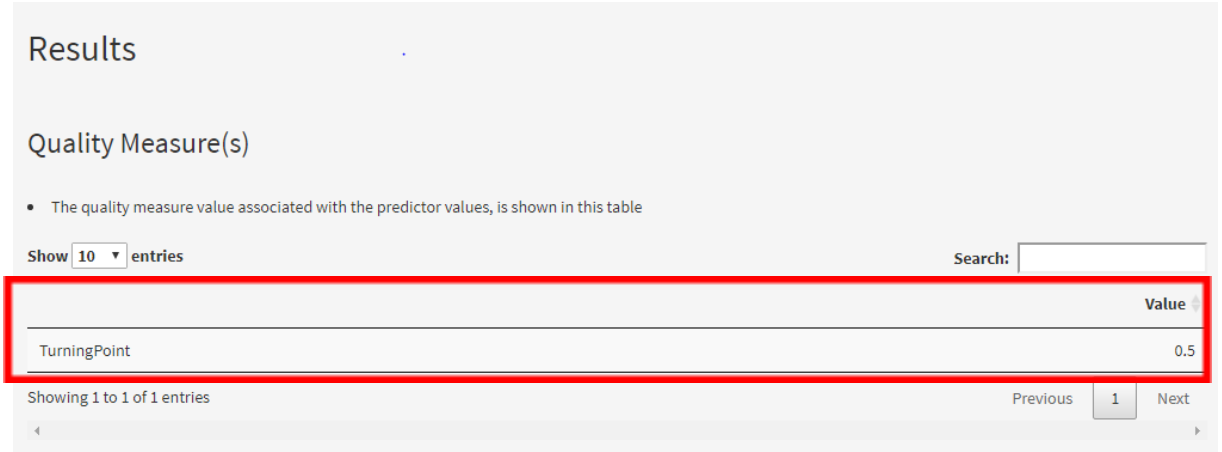
### *Linear Optimisation*



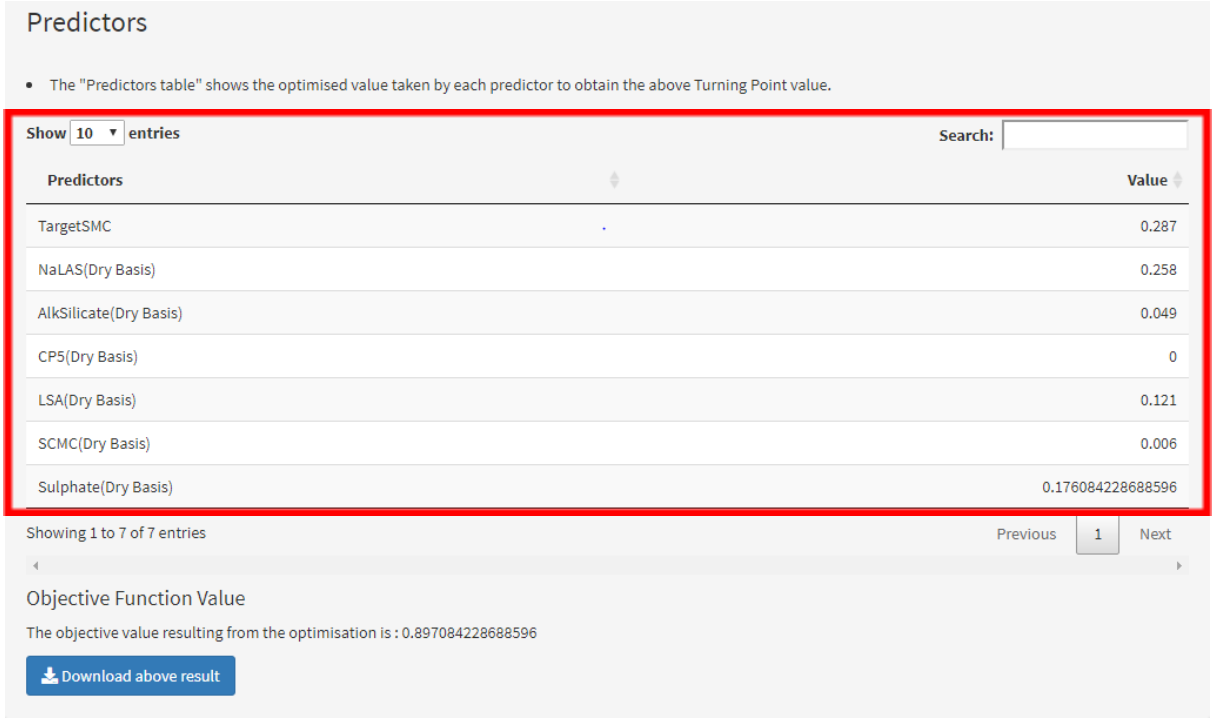

- This solution can be constrained by minimizing and maximizing an objective function.
- The optimal solution is calculated by setting up and solving the associated linear programming problem using the R package "lpSolveAPI". Suppose there is a quality measure R and predictors P1, P2,..., Pn. A linear program is set as below.
    - minimize or maximize the objective function: $\sum CiPi$ ; where $Ci$ refers to the objective function coefficient for the predictor $Pi$.
    - quality measure achieves a target value or range : $R \leq t, R = t$ or $R \geq t$.
    - predictors lie within specified limits : $Li \leq Pi \leq Ui$ ; where $Li$ and $Ui$ are the lower and upper bounds of predictor $Pi$.
- Select minimization or maximization as per need by clicking on the checkbox in the red box.
- Select the desired inequality from "less than or equal to", "equal to" and "greater than or equal to"




- The first column shows the predictor names along with their expected lower and upper bounds which are given in the brackets
- Obj_coeff column is set to a default at 1 and is used for assigning weights to each predictor
- Change the lower and upper bounds of the predictor variable
- Once the changes are made click on “Run Optimiser”

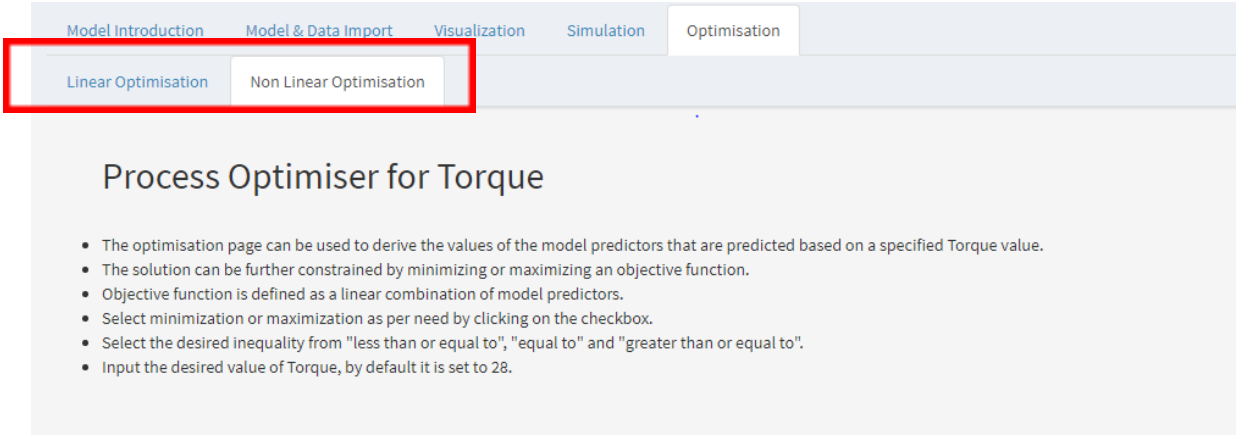



- The results table shows the Predicted Value of the response variable



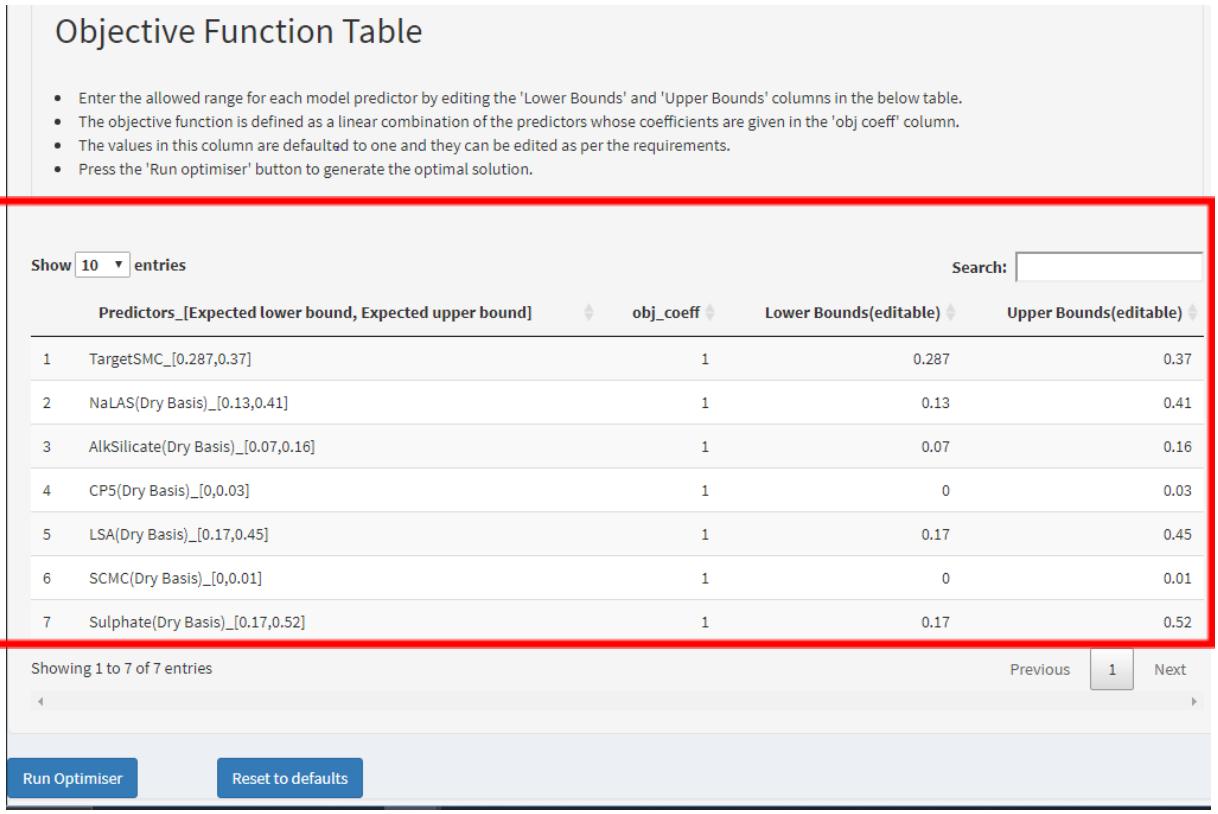

- The predictors table show the value taken by each predictor to obtain the Predicted Response variable value
- “Download Above results” the downloads outcome of Linear Optimisation

## *Non-Linear Optimisation*

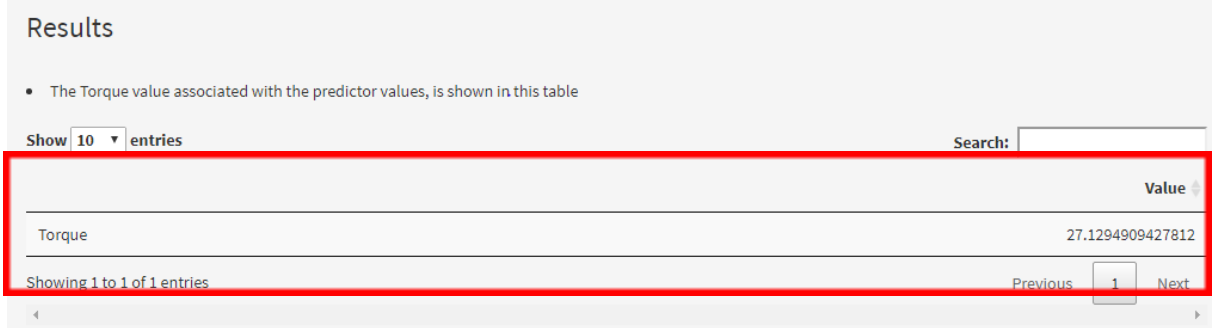



- The red box shows selection as non-linear
- All the non-linear equations within the model are optimised here

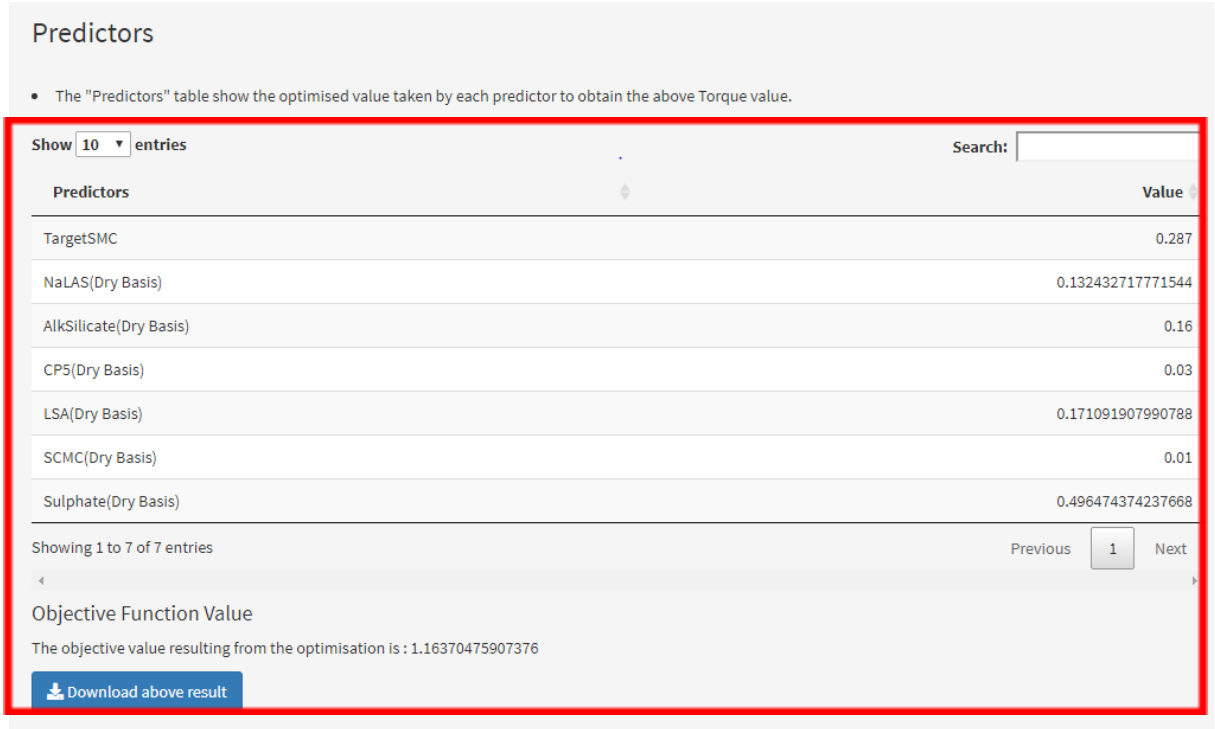

- This solution can be constrained by minimizing and maximizing an objective function.
- The optimal solution is calculated by setting up and solving the associated non-linear programming problem using the R package "nloptr". Suppose there is a quality measure R and predictors P1, P2, P3; let the associated non linear equation be R = P1 + P2*P3 . A linear program is set as below.
    - minimize or maximize the non-linear objective function: C1*P1 + (C2*P2)*(C3*P3) ; where $Ci$ refers to the objective function coefficient for the predictor $Pi$; in other words, the regression coefficients in the equation are replaced by the respective weights of the predictor variables and the non-linear objective function is formulated.
    - quality measure achieves a target value or range : $R \leq t, R = t$ or $R \geq t$.
    - predictors lie within specified limits : $Li \leq Pi \leq Ui$ ; where $Li$ and $Ui$ are the lower and upper bounds of predictor $Pi$.
- Select minimization or maximization as per need by clicking on the checkbox in the red box.
- Select the desired inequality from "less than or equal to", "equal to" and "greater than or equal to"



- The first column shows the predictor names along with their expected lower and upper bounds which are given in the brackets
- Obj_coeff column is set to a default at 1 and is used for assigning weights to each predictor
- Change the lower and upper bounds of the predictor variable
- Once the changes are made click on “Run Optimiser”

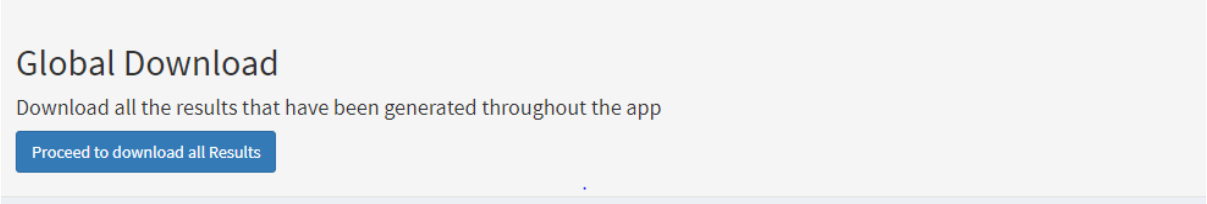


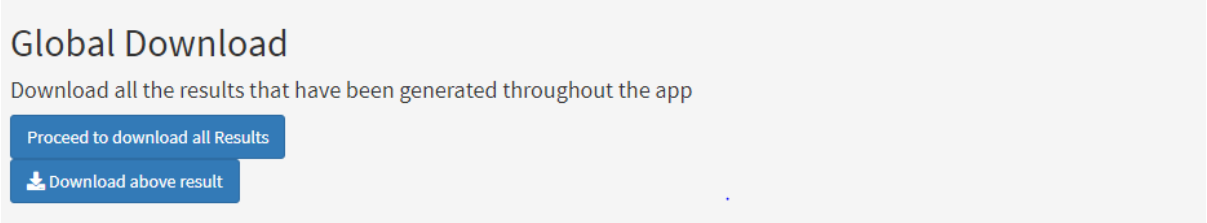

- The results table shows the Predicted Value of the response variable




- The predictors table show the value taken by each predictor to obtain the Predicted Response variable value
- Download above results saves the results generated from non-linear optimisation

## Global Download




- Press on proceed to download all Results
- The “Download above Results.” Will appear, click on that
- Global download allows the user to download all the results that is manual entry simulation, import data simulation and the results of optimization.
- Please note that only results that are generated will be downloaded.