

# 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

The screenshot displays the 'Model Bank Functionalities' section with a list of five bullet points. Below this is a horizontal navigation bar with five tabs: 'Model Introduction', 'Model & Data Import', 'Visualization', 'Simulation', and 'Optimisation'. The 'Model Introduction' tab is highlighted with a red rectangular box. Below the navigation bar, the 'Home Care Slurry Viscosity Drying Model' is displayed, including its owners (Amanda Iane, Aditi Mahajan), a description of the model's purpose, and a detailed note about ingredient reporting.

**Model Bank Functionalities**

- The application has models built in itself already and allows user to select one for further exploration.
- Import of new simulation data is possible. User can input simulation values as well.
- Visualization tab provides visual guide of the imported simulation data.
- Simulation tab allows for simulation of selected models on the imported data or input values.
- Optimisation tab helps to optimise the models and draw meaningful insights.

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

### Home Care Slurry Viscosity Drying Model

*Model Owners: Amanda Iane, Aditi Mahajan*

This model uses the slurry composition to predict slurry viscosity (Torque) and the ease of drying and provide recommendations for optimal slurry composition.

The viscosity and dry-ability of slurries for spray dried laundry powders have been found to be closely related to the formulation composition. As a result, the Home Care Slurry Viscosity Drying Model has been developed, through a design of experiments, to predict slurry viscosity and slurry dry-ability as a function of slurry composition.

**Note - All ingredients (except target slurry moisture content i.e. Target SMC) should be reported as fractions on a dry basis (w/w). Sum of all dry ingredient should be = 1 Target SMC should be reported as a fraction on the wet slurry basis (w/w)**

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

## 2 -Model and Data Import:

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

### Available Model Outputs

- This table presents the available model for this segment.
- Simulation will take place for both equations simultaneously.
- Variables used in Torque, except TargetSMC, are derived variables e.g. NaLASnew = (NaLAS (dry basis)/Sum)\*(1-TargetSMC)
- Sum = NaLAS (dry basis) + AlkSilicate (dry basis) + LSA (dry basis) + CP5 (dry basis) + SMC (dry basis) + Sulphate (dry basis)

Show  entries   Search:

	Models
1	Torque := 550.942517169757 *TargetSMC + 657.293920443309 *NaLASnew + -178.742137567497 *AlkSilicatenew + -145.925867640988 *CP5new +484.822800006602 *LSAnew + 205.55728325435 *SCMCnew + 14.7480644403947 *Sulphatenew + -435.366522312941 *0 + TargetSMC * (NaLASnew *-2509.30663159213) +TargetSMC * (Sulphatenew * -909.820229343898) +TargetSMC * (LSAnew * -2140.43715033235)
2	TurningPoint := 1.64652727504537*TargetSMC + -0.340054974118285*NaLAS + 0.0349876142645199*AlkSilicate + -0.26064073764549*CP5 + -0.0575389664392278*LSA + -1.17237663840093*SCMC + -0.298363251134605*Sulphate

Showing 1 to 2 of 2 entries   Previous   **1**   Next

- 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.

**Accepted range for user inputs**

Show  entries   Search:

	Ingredients	Lower_Level	Upper_Level
1	TargetSMC	0.287	0.37
2	NaLAS (dry basis)	0.13	0.41
3	Alkaline Silicate (dry basis)	0.07	0.16
4	Sodium Carbonate (dry basis)	0.17	0.45
5	CP5 (dry basis)	0	0.03
6	SCMC (dry basis)	0	0.01
7	Sodium Sulphate (dry basis)	0.17	0.52

Showing 1 to 7 of 7 entries   Previous   **1**   Next

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

## 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](#)

- Following table is editable. Enter the simulation values.
- Entered values will automatically be saved for simulation stage.
- Target Slurry Moisture Content denotes the fraction of water in the slurry.
- All other ingredient content must be reported on dry basis.
- Measurement Units of all variables are in fractions i.e. 0-1. User must follow these limits.

Show 10 entries

Search:

	TargetSMC	NaLAS (dry basis)	AlkSilicate (dry basis)	LSA (dry basis)	CP5 (dry basis)	SCMC (dry basis)	Sulphate (dry basis)
Enter Simulation Values	0.287	0.13	0.07	0.17	0	0	0.17

Showing 1 to 1 of 1 entries

Previous 1 Next

[Go to simulation](#)

- 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**

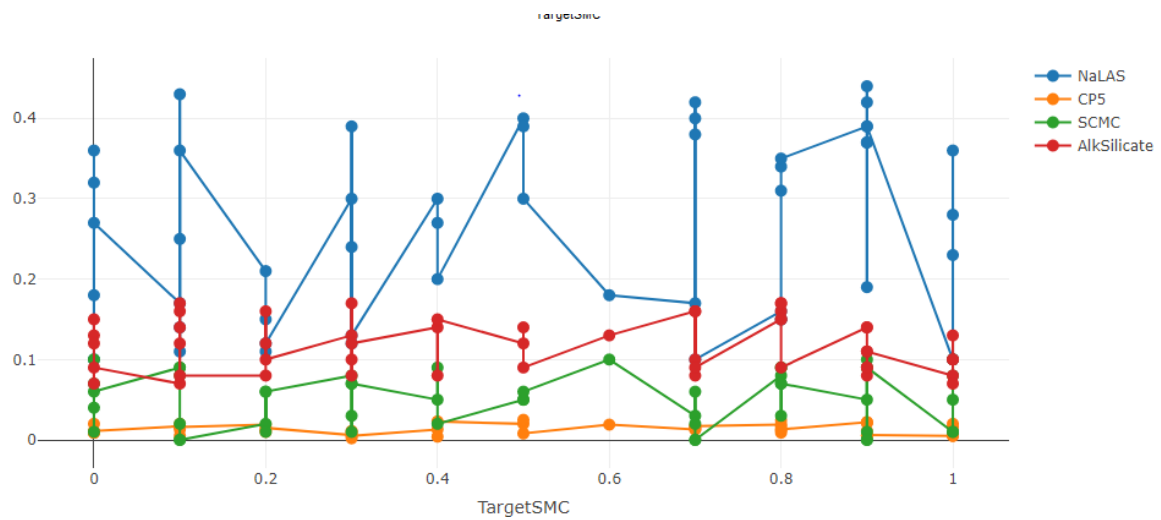
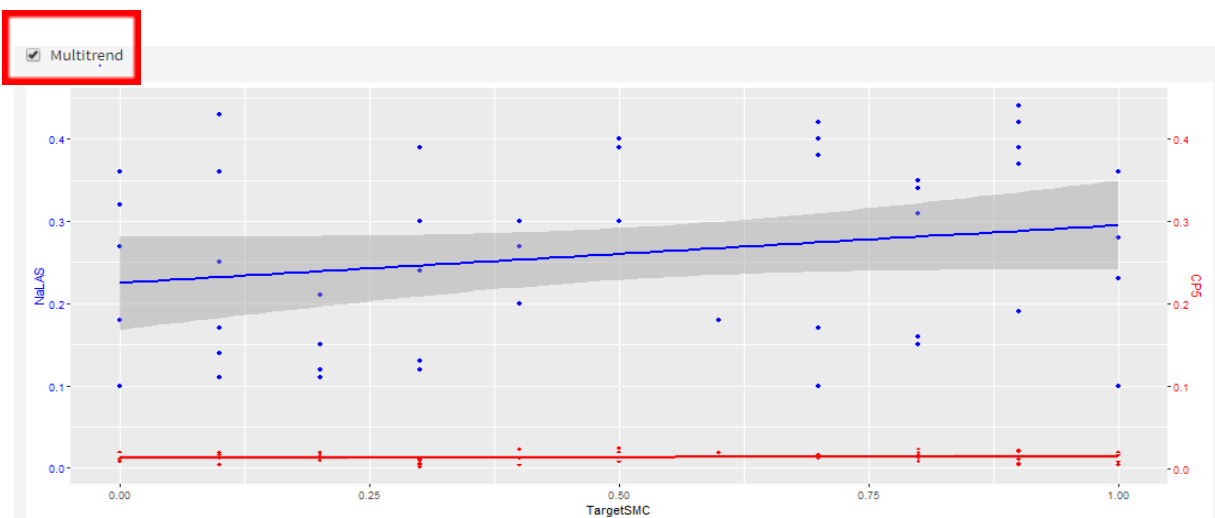
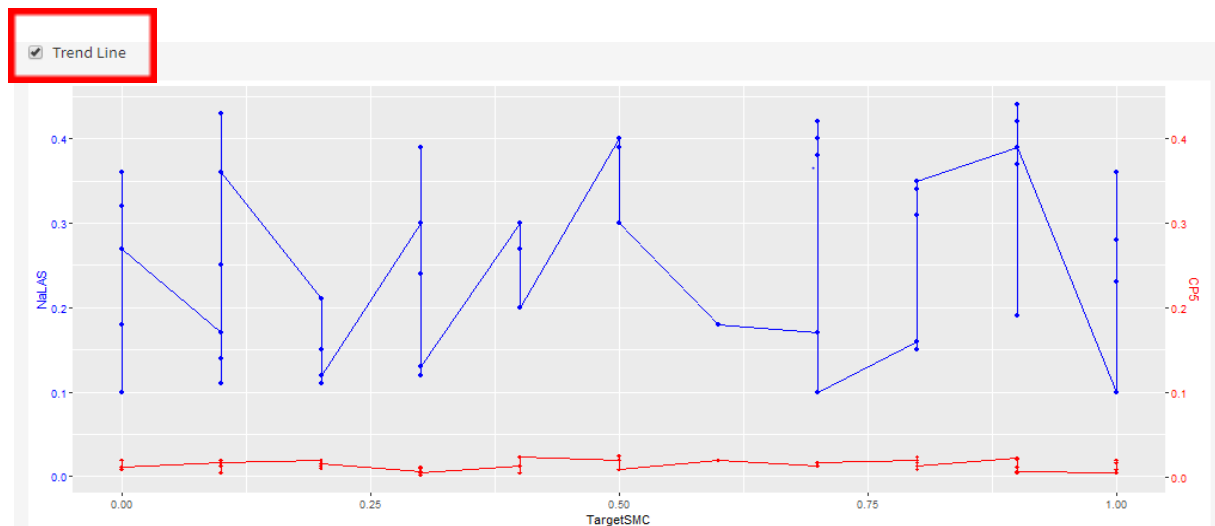
TargetSMC

**Y axis**

NaLAS

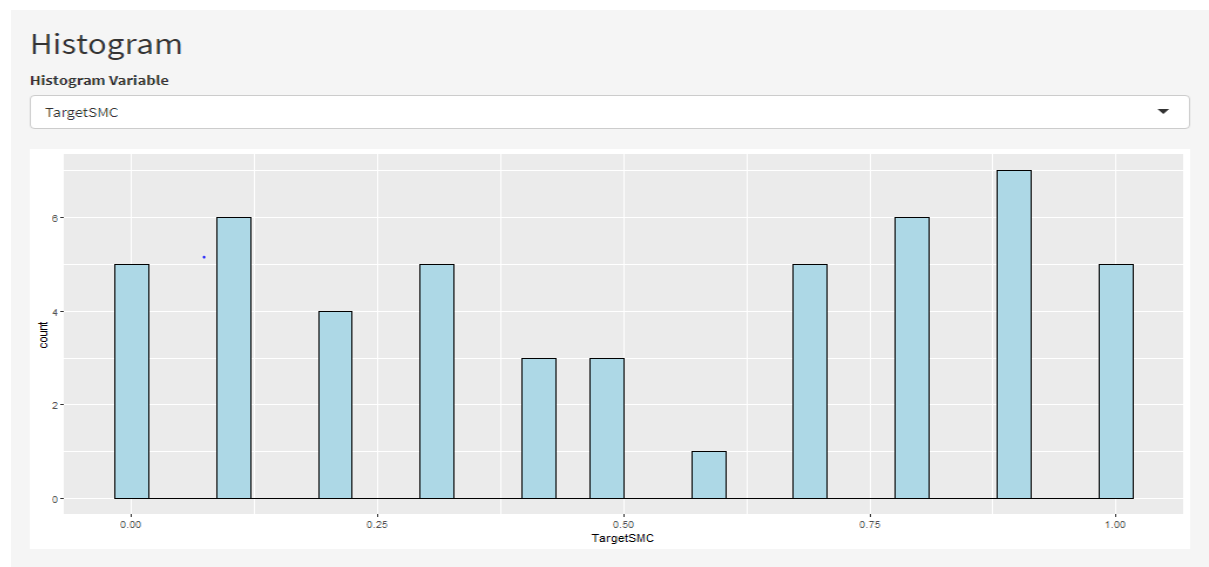
- First two graphs allow for double Y axis selection with single x axis.
- It takes the first two selections of y-axis for plotting. Linear regression method is used for creating trendlines in second graph.
- Checkboxes can be used for adding or removing the trends in graph.

- 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)

Model IntroductionModel & Data ImportVisualizationSimulationOptimisation

Simulation Input Response

Manual Entry SimulationProfilerImported Data Simulation

Input values taken for manual simulation

Show 10 entries

Search:

	TargetSMC	NaLAS (dry basis)	AlkSilicate (dry basis)	LSA (dry basis)	CP5 (dry basis)	SCMC (dry basis)	Sulphate (dry basis)
Enter Simulation Values	0.287	0.35	0.07	0.39	0.01	0.01	0.17

Showing 1 to 1 of 1 entries

Previous1Next

Simulate on entered Data

Calculated Values for New Variables

Show 10 entries

Search:

	NaLASnew	AlkSilicatenew	CP5new	LSAnew	SCMCnew	Sulphatenew
1	0.25	0.05	0.007	0.278	0.007	0.121

Showing 1 to 1 of 1 entries

Previous1Next

Predicted Values and their Classification

Show 10 entries

Search:

Torque	TurningPoint	ClosestFriend	Dryability
68.0658853766532	0.268491096630492	SRC12.5	Green

Showing 1 to 1 of 1 entries

Previous1Next

Torque value should be between 19 & 36. Above value is out of bounds.

- 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.



Show 11 entries Search:

	Easy(1)	Easy(2)	Easy(3)	Easy(4)	Hard(5)	Hard(6)	Hard(7)	Very_Hard(8)	Very_H
P45									
P42								X	
H35								X	
F40								X	
M30					X				
M25					X				
M20					X				
SRG20	X								
C53	X								
SRC13.5	X								
SRC12.5 ✓									

Showing 1 to 11 of 11 entries Previous 1 Next

Download above result

- 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

### Simulation Input Response

Manual Entry Simulation

Profiler

Imported Data Simulation

## Profiler

### Dryability Classification of Slurry

Show 11 entries

Search:

Easy(1)

Easy(2)

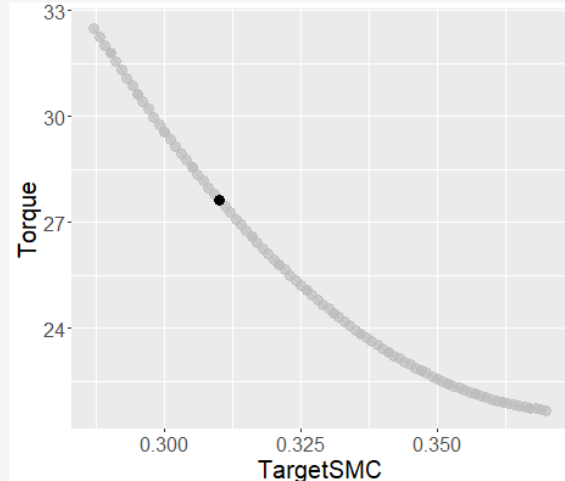
Easy(3)

Easy(4)

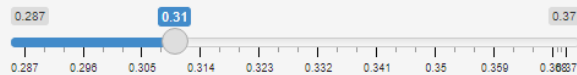
Hard(5)

P45					
P42					
F40					
H35					
M30					
M25					
M20					X
SRG20				X	
C53			X		

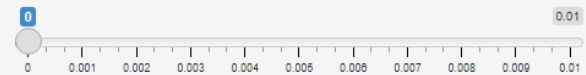
### Torque



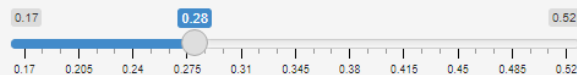
TargetSMC:



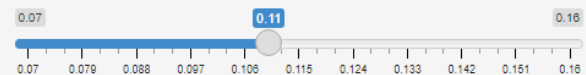
SCMC (dry basis):



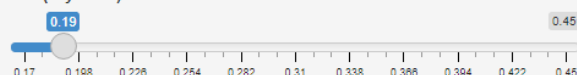
Sulphate (dry basis):



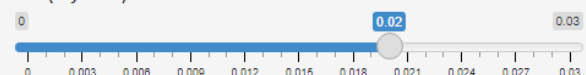
Alkaline Silicate (dry basis):



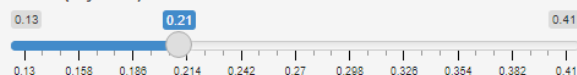
LSA (dry basis):



CP5 (dry basis):



NaLAS (dry basis):



- 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

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

### Simulation Input Response

Manual Entry Simulation   Profiler   Imported Data Simulation

Table only presents the results with condition of predicted Torque being in the range of 19 to 36.

[Simulate on Imported Data](#)

- 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

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

### Simulation Input Response

Manual Entry Simulation   Profiler   Imported Data Simulation

Table only presents the results with condition of predicted Torque being in the range of 19 to 36.

[Simulate on Imported Data](#)

#### Predicted Values and their Classification

Show  entries   Search:

	Torque	TurningPoint	ClosestFriend	Dryability
37	35.0570441567846	0.503238830669561	F40	Red (Very Hard)

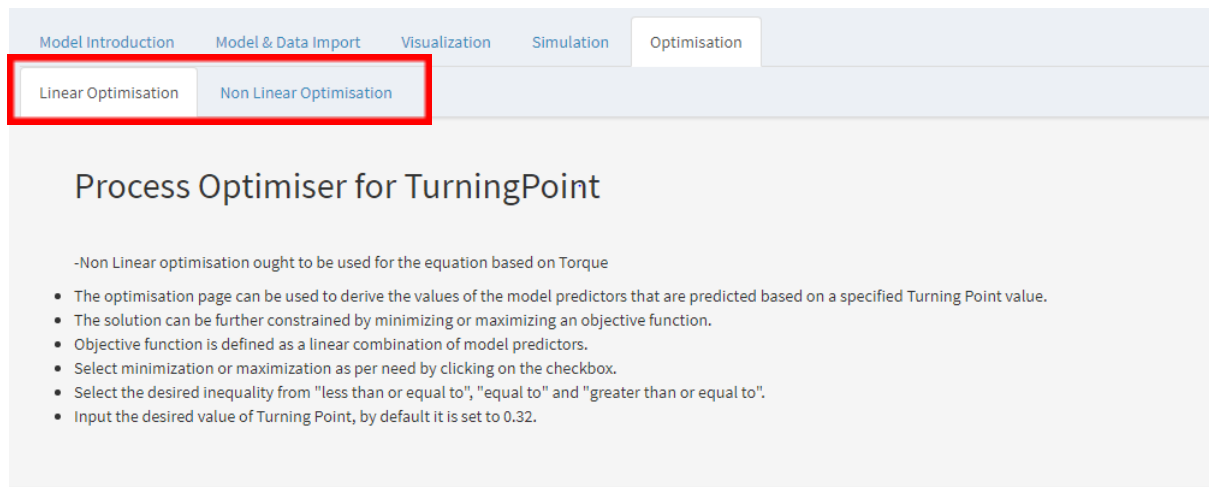
Showing 1 to 1 of 1 entries   Previous      Next

[Download above result](#)

- “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.



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

**Linear Optimisation**   Non Linear Optimisation

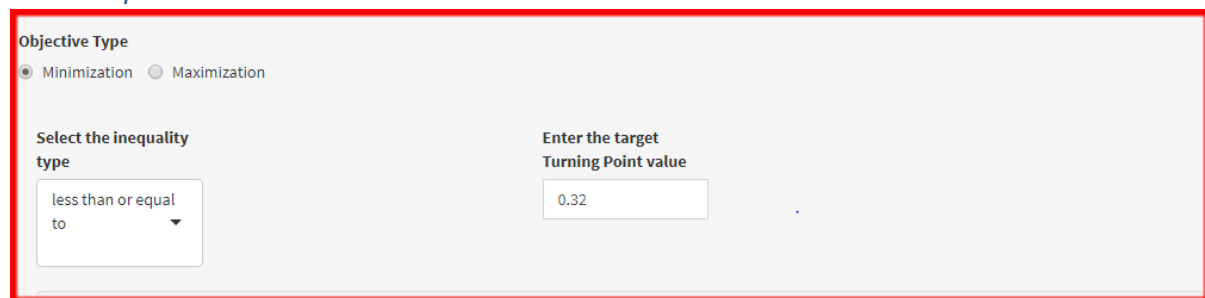
### Process Optimiser for TurningPoint

-Non Linear optimisation ought to be used for the equation based on Torque

- The optimisation page can be used to derive the values of the model predictors that are predicted based on a specified Turning Point value.
- The solution can be further constrained by minimizing or maximizing an objective function.
- Objective function is defined as a linear combination of model predictors.
- Select minimization or maximization as per need by clicking on the checkbox.
- Select the desired inequality from "less than or equal to", "equal to" and "greater than or equal to".
- Input the desired value of Turning Point, by default it is set to 0.32.

- 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



**Objective Type**

☒ Minimization   ☐ Maximization

**Select the inequality type**

less than or equal to

**Enter the target Turning Point value**

0.32

- 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  $P_1, P_2, \dots, P_n$ . A linear program is set as below.
  - minimize or maximize the objective function:  $\sum C_i P_i$  ; where  $C_i$  refers to the objective function coefficient for the predictor  $P_i$ .
  - quality measure achieves a target value or range :  $R \leq t, R = t$  or  $R \geq t$ .
  - predictors lie within specified limits :  $L_i \leq P_i \leq U_i$  ; where  $L_i$  and  $U_i$  are the lower and upper bounds of predictor  $P_i$ .
- 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"

## Objective Function Table

- Enter the allowed range for each model predictor by editing the 'Lower Bounds' and 'Upper Bounds' columns in the below table.
- The objective function is defined as a linear combination of the predictors whose coefficients are given in the 'obj coeff' column.
- The values in this column are defaulted to one and they can be edited as per the requirements.
- Press the 'Run optimiser' button to generate the optimal solution.

Show10▼entries

Search:

	Predictors_[Expected lower bound, Expected upper bound]	obj_coeff	Lower Bounds(editable)	Upper Bounds(editable)
1	TargetSMC_[0.287,0.37]	1	0.287	0.37
2	NaLAS(Dry Basis)_[0.13,0.41]	1	0.13	0.41
3	AlkSilicate(Dry Basis)_[0.07,0.16]	1	0.07	0.16
4	CP5(Dry Basis)_[0,0.03]	1	0	0.03
5	LSA(Dry Basis)_[0.17,0.45]	1	0.17	0.45
6	SCMC(Dry Basis)_[0,0.01]	1	0	0.01
7	Sulphate(Dry Basis)_[0.17,0.52]	1	0.17	0.52

Showing 1 to 7 of 7 entries

Previous1Next

Run Optimiser

Reset to defaults

- 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”

## Results

### Quality Measure(s)

- The quality measure value associated with the predictor values, is shown in this table

Show

10

entries

Search:

	Value
TurningPoint	0.5

Showing 1 to 1 of 1 entries

Previous

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Next

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

### Predictors

- The "Predictors table" shows the optimised value taken by each predictor to obtain the above Turning Point value.

Show **10** entries Search:

Predictors	Value
TargetSMC	0.287
NaLAS(Dry Basis)	0.258
AlkSilicate(Dry Basis)	0.049
CP5(Dry Basis)	0
LSA(Dry Basis)	0.121
SCMC(Dry Basis)	0.006
Sulphate(Dry Basis)	0.176084228688596

Showing 1 to 7 of 7 entries Previous **1** Next

Objective Function Value

The objective value resulting from the optimisation is : 0.897084228688596

[Download above result](#)

- 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

Model Introduction Model & Data Import Visualization Simulation Optimisation

Linear Optimisation Non Linear Optimisation

### Process Optimiser for Torque

- The optimisation page can be used to derive the values of the model predictors that are predicted based on a specified Torque value.
- The solution can be further constrained by minimizing or maximizing an objective function.
- Objective function is defined as a linear combination of model predictors.
- Select minimization or maximization as per need by clicking on the checkbox.
- Select the desired inequality from "less than or equal to", "equal to" and "greater than or equal to".
- Input the desired value of Torque, by default it is set to 28.

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

**Objective Type**  
☒ Minimization ☐ Maximization

Select the inequality type  
 less than or equal to

Enter the target Torque value  
 28

- 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  $P_1, P_2, P_3$ ; let the associated non linear equation be  $R = P_1 + P_2 * P_3$ . A linear program is set as below.
  - o minimize or maximize the non-linear objective function:  $C_1 * P_1 + (C_2 * P_2) * (C_3 * P_3)$ ; where  $C_i$  refers to the objective function coefficient for the predictor  $P_i$ ; 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.
  - o quality measure achieves a target value or range :  $R \leq t, R = t$  or  $R \geq t$ .
  - o predictors lie within specified limits :  $L_i \leq P_i \leq U_i$ ; where  $L_i$  and  $U_i$  are the lower and upper bounds of predictor  $P_i$ .
- 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”

### Objective Function Table

- Enter the allowed range for each model predictor by editing the 'Lower Bounds' and 'Upper Bounds' columns in the below table.
- The objective function is defined as a linear combination of the predictors whose coefficients are given in the 'obj coeff' column.
- The values in this column are defaulted to one and they can be edited as per the requirements.
- Press the 'Run optimiser' button to generate the optimal solution.

Show	10	entries	Search: <input type="text"/>		
	Predictors_[Expected lower bound, Expected upper bound]	obj_coeff	Lower Bounds(editable)	Upper Bounds(editable)	
1	TargetSMC_[0.287,0.37]	1	0.287	0.37	
2	NaLAS(Dry Basis)_[0.13,0.41]	1	0.13	0.41	
3	AlkSilicate(Dry Basis)_[0.07,0.16]	1	0.07	0.16	
4	CP5(Dry Basis)_[0,0.03]	1	0	0.03	
5	LSA(Dry Basis)_[0.17,0.45]	1	0.17	0.45	
6	SCMC(Dry Basis)_[0,0.01]	1	0	0.01	
7	Sulphate(Dry Basis)_[0.17,0.52]	1	0.17	0.52	

Showing 1 to 7 of 7 entries
 

Previous
 1
 Next

Run Optimiser

Reset to defaults

- 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”

### Results

- The Torque value associated with the predictor values, is shown in this table

Show  entries Search:

	Value
Torque	27.1294909427812

Showing 1 to 1 of 1 entries Previous  Next

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

### Predictors

- The "Predictors" table show the optimised value taken by each predictor to obtain the above Torque value.

Show  entries Search:

Predictors	Value
TargetSMC	0.287
NaLAS(Dry Basis)	0.132432717771544
AlkSilicate(Dry Basis)	0.16
CP5(Dry Basis)	0.03
LSA(Dry Basis)	0.171091907990788
SCMC(Dry Basis)	0.01
Sulphate(Dry Basis)	0.496474374237668

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#### Objective Function Value

The objective value resulting from the optimisation is : 1.16370475907376

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- The predictors table show the value taken by each predictor to obtain the Predicted Response variable value
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## Global Download

### Global Download


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