Documentation

Contents

Documentation 1
- Run simulation 2
- Experiments 3
  - Experiment profile (Not Editable) 3
  - Experiments Data (Not editable) 4
  - Simulation Data Setting – “Name configuration” 4
- Dataset 5
  - Raw Materials 5
  - Master Conditions 5
  - Exp Unit Conditions 5
  - Master Outcomes 6
  - Exp Unit Outcomes 6
- Report 7
  - Inputs 7
  - Key results 7
  - Process diagram 7
  - Assumptions 7
  - Recommendations 7
  - Simulation notes 7
- Release note 8
- Roadmap 8
- Support 8

Last updated: 5 July 2021

Run simulation

- Step 1: Go to Experiments – Experiments. Existing experiments are listed in this page. (Figure 1)
- Step 2: Click on the gear icon of an experiment and select 'Manage'. (Figure 1)
- Step 3: Click on 'View Configurations'. Saved configurations will be listed.(Figure 2)
- Step 4: Click on the gear button of a configuration and select 'View Data Set'. (Figure 2)
- Step 5: Edit the values by clicking the edit button. (If you want to edit existing dataset, click 'View Dataset'. Click the Gear icon of the dataset that you want to edit and select 'Edit'.)
- Step 6: Save the values as a dataset by clicking 'Save Current Dataset' and give a name to the new dataset. (Figure 3)
- Step 7: In the saved dataset list, click the gear button of the dataset that you want to use for the simulation and select 'Simulate Output'. Give a name to the report that will be generated. (Figure 3)
- Step 8: Go to Reports – Experiment and check the status of the experiment that is executed. (Figure 4)
- Step 9: If the status is 'Success', click on the gear button and select 'View'. (Figure 4)

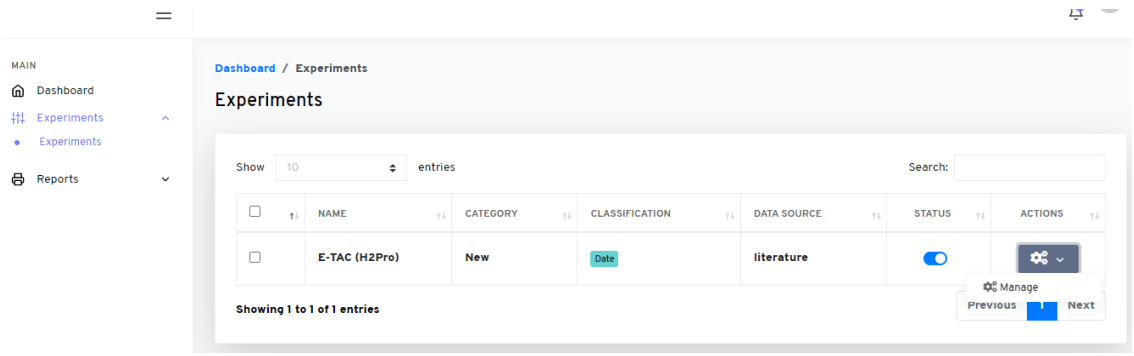

Figure 1: list of experiments

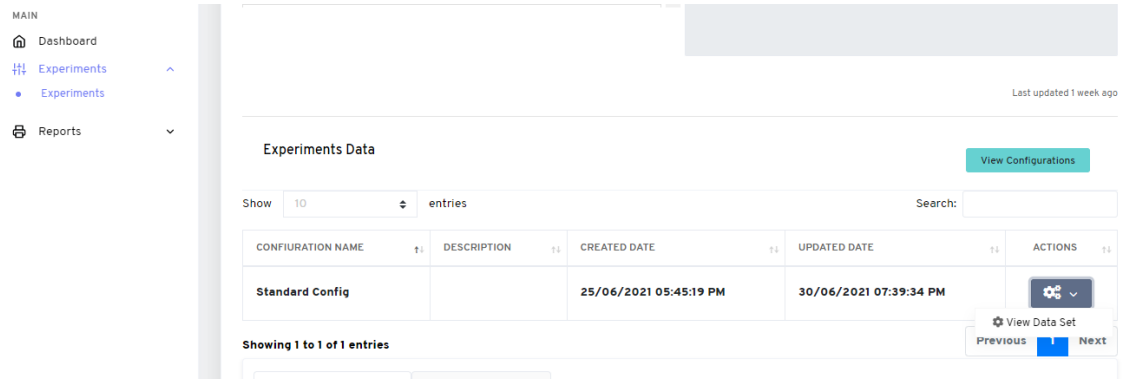

Figure 2 List of configurations

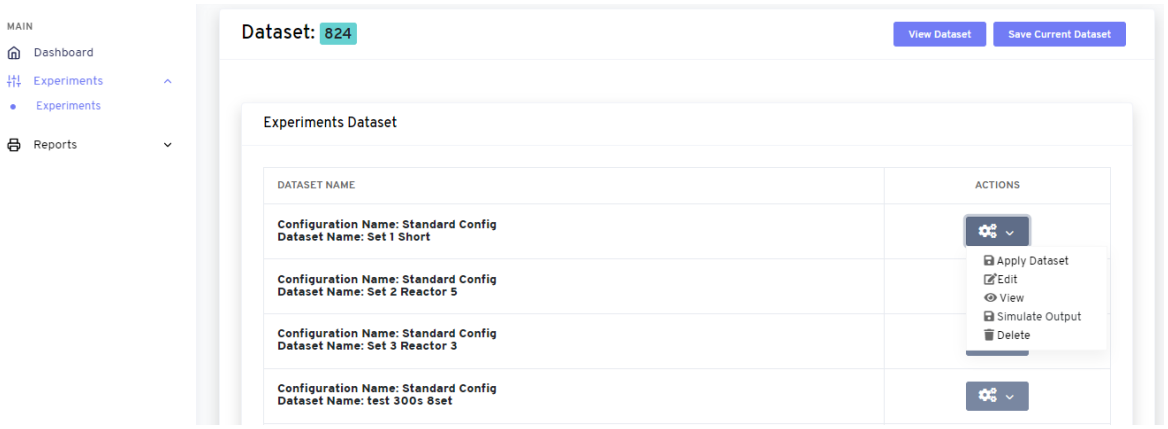

Figure 3 List of datasets

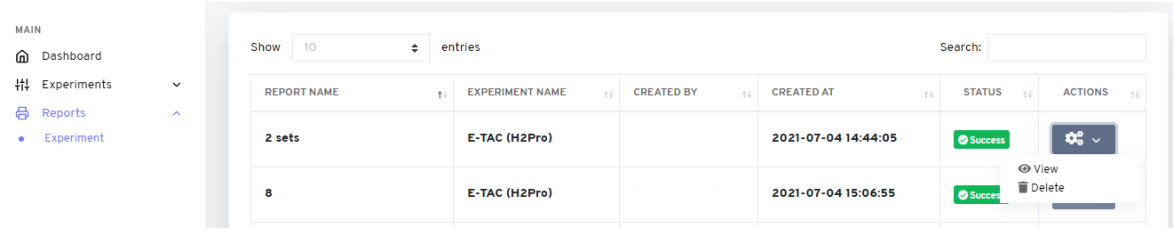

Figure 4 list of reports

Experiments

Experiments is the section which describes the process model and the section to execute the simulation.

Experiment profile (Not Editable)

This table describes the basic information of the experiment.

Category: describes whether the experiment is created for a new process or an old process.

Classification: describes how the dataset are collected.

Data Source: source of the information used to create the model

Selected Experiments Units: experiment unit name and the respective models (highlighted in blue)

Selected Products: chemicals/products present in the experiments

Selected Energy Utilities: utility type used in the experiment

Main Product Input: raw material of the experiment which is selected from 'Selected Products'

Main Product output: desired product of the experiment which is selected from 'Selected Products'

Tags: keyword assigned to the experiment

Description: description of the experiment

Experiments Data (Not editable)

Experiments data contains the information on the process. The connections between the experiment units and the process flow diagram of the process are visible under the tab 'Process Flow Diagram'. Conditions relevant to the units, experimental outcomes calculated in each unit and reactions occurring at each unit are given under the tab 'Unit Specifications'. The defined 'Process Flow Diagram' and 'Unit Specifications' can be saved as configuration and can be used for the simulation.

Process Flow Diagram

The stream table describes how the streams are connected. Process flow diagram will be created based on the streams defined in the stream table. Currently, the stream table and the process flow diagram are fixed and are not editable.

The stream table provides the following information:

SERIAL No: stream number as shown in the process flow diagram

PFD STREAM NAME: stream name as defined in the experiments

FROM UNIT>EXPERIMENT UNIT: describes where the stream comes from. It is an output stream of the selected unit. If this is empty, the stream is an open input stream.

FROM UNIT>EXPERIMENT STREAM: stream name corresponding to the unit model. Number of output stream for each unit model is predefined.

TO UNIT>EXPERIMENT UNIT: describes where the stream flow to. It is an input stream to the selected unit. If this is empty, the stream is an open output stream.

FROM UNIT>EXPERIMENT STREAM: stream name corresponding to the unit model. Number of input stream for each unit model is predefined.

STREAM FLOW TYPE: description of the stream type

ACTIONS: one can edit or delete a stream

Unit Specifications

This tab has a sub tab of 'Master Data' and units defined in 'Selected Experiments Units'. For each sub tab, the user can select the conditions, outcomes and reactions relevant to the particular master data/unit. 'Master Data' is the tab for the entire system.

View Configurations

Given information on process flow diagram and unit specifications can be stored as a configuration. 'View Configurations' will list all the stored configurations. By selecting 'View Data Set', the user can jump to the window where the values can be added to the selected conditions and execute the simulation.

Simulation Data Setting – "Name configuration"

This page is to add value to the defined condition in the previous configuration step. One has to save the given values as a dataset. Simulation can only be executed for a dataset that has been stored.

Simulate Output – Forward Model

This tab is to add value for the forward simulation, i.e. the user can add values to the conditions defined in the configuration and by executing the simulation, one can get the values for the outcomes for the defined time operating time. 'Simulate Output – Forward Model' is composed of 5 sub tabs:

Raw materials: product and mass flow rate can be defined for open input streams

Master Condition: One can define value and unit for the master condition. Unit conversion is not working yet. Please only change the value.

Exp Unit Conditions: One can add value and unit for the experiment unit condition. Unit conversion is not working yet. Please only change the value.

Master Outcomes: one can select the unit of measurement for master outcomes. Unit conversion is not working yet. Changing the unit will not change the result.

Exp Unit Outcomes: one can select the unit of measurement for experiment unit outcome, but unit conversion is not working yet. Changing the unit will not change the result.

Dataset

Raw Materials

H2O-in : Input stream to hot tank in ton/second

Master Conditions

CONDITION	UNIT	DESCRIPTION
Operating Time	S	Duration of the simulation
Current	A	Applied current over the system
time interval	S	Amount of time between the calculation

Exp Unit Conditions

EXPERIMENT UNIT NAME	CONDITION	UNIT	DESCRIPTION
red_tank	Volume	m^3	Volume of hot tank
red_tank	Temperature	C	Set temperature of hot tank
red_tank	Pressure	Pa	Set pressure of hot tank
red_tank	Volumetric Flow	m^3/h	Recycle flow to hot tank
red_tank	Volume Level	-	Volume level in hot tank
red_tank	diameter	m	Diameter of hot tank
red_tank	outlet diameter	m	Outlet diameter of hot tank
red_tank	Initial height	m	Initial liquid level in hot tank
red_tank	Initial pressure	Pa	Initial gas pressure in hot tank
grey_tank	Volume	m^3	Volume of wash tank
grey_tank	Temperature	C	Set temperature of wash tank
grey_tank	Pressure	Pa	Set pressure of wash tank
grey_tank	Volumetric Flow	m^3/h	Recycle flow to wash tank
grey_tank	Volume Level	-	Volume level in wash tank
grey_tank	diameter	m	Diameter of wash tank
grey_tank	outlet diameter	m	Outlet diameter of wash tank
grey_tank	Initial height	m	Initial liquid level in wash tank
grey_tank	Initial pressure	Pa	Initial gas pressure in wash tank
blue_tank	Volume	m^3	Volume of cold tank

Last updated: 5 July 2021

blue_tank	Temperature	C	Set temperature of cold tank
blue_tank	Pressure	Pa	Set pressure of cold tank
blue_tank	Volumetric Flow	m^3/h	Recycle flow to cold tank
blue_tank	Volume Level	-	Volume level in cold tank
blue_tank	diameter	m	Diameter of cold tank
blue_tank	outlet diameter	m	Outlet diameter of cold tank
blue_tank	Initial height	m	Initial liquid level in cold tank
blue_tank	Initial pressure	Pa	Initial gas pressure in cold tank
heater	Temperature	C	Desired temeperature after heater
heater	max power	kW	Maximum power input of the heater
roll	Volume	m^3	Volume of one roll
roll	Electrode area	m^2	Electrode area in a roll
roll	Voltage	V	Initial voltage of a roll
roll	Current	A	Initial current of a roll
roll	Initial mass	Kg	Initial mass in a roll
set	n_set	-	Number of set in the system
set	n_reactor	-	Number of reactor in a set
set	n_roll	-	Number of roll in a reactor
Step	'H' step duration	s	Duration of 'H' step
Step	'H with no current' step duration (before)	s	Duration of 'H' step without current before current has been appli
Step	'H with no current' step duration (after)	s	Duration of 'H' step without current after current has been applied
Step	'W' step duration	s	Duration of 'W' step
Step	'O' step duration	s	Duration of 'O' step
Step	Step transition duration	s	Duration of the transition step between different steps
Step	Step shift	s	Time shift between different set
pump-blue	Efficiency	-	Pump efficiency for the pump connected to cold tank
pump-grey	Efficiency	-	Pump efficiency for the pump connected to wash tank
pump-red	Efficiency	-	Pump efficiency for the pump connected to hot tank
cooler	Temperature	C	Desired temperature after cooler
cooler	max power	W	Maximum power input for the cooler

Master Outcomes

OUTCOME	UNIT	DESCRIPTION
Power	Kw	Power of the system
H2 production	kg/day	Hydrogen production of the system
Current	A	Current over the system
Voltage	V	Applied voltage of the system

Exp Unit Outcomes

EXPERIMENT NAME	OUTCOME	UNIT	DESCRIPTION
red_tank	gas residual	w%	percentage of H_2 and O_2 in the gas phase in the hot tank
grey_tank	gas residual	w%	percentage of H_2 and O_2 in the gas phase in the wash tank
blue_tank	gas residual	w%	percentage of H_2 and O_2 in the gas phase in the cold tank

Last updated: 5 July 2021

Report

The outcome of the executed simulation can be viewed in the report. It has the following tabs: Inputs, Key results, Process diagram, Assumptions, Recommendations and Simulation notes. The Inputs and the Key results will have two tabs: Summary and Detailed.

Inputs

This tab shows the conditions used to execute the simulation. The summary tab shows Master Conditions. Detailed tab shows the values defined in Exp Unit Conditions and Raw Materials.

Key results

This tab shows the outcome of the executed simulation. The summary tab will show the result of the Master Outcomes. The Detailed tab shows the result of Exp Unit Outcomes, stream data and graphs.

Process diagram

This tab shows the process flow diagram of the experiment.

Assumptions

This tab lists the assumptions used to create the models.

Recommendations

This tab lists the recommendations to improve the accuracy and the quality of the models.

Simulation notes

If error occurs, this tab should be highlighted to show user that something is wrong with the inputs provided.

Release note

Unit conversion module is not implemented. When changing the value in the application, unit can be changed, but this will not affect the results. The units used in the calculation are listed in Dataset.

Some combination of n_set, n_reactor and n_roll in Exp unit conditions will throw an error and the report will not be generated.

In case the report is not generated properly, it should show failed and the error message should be shown in Simulation notes. Currently it stays as pending and the report cannot be viewed

Graphs for energy losses will be added in the report section.

Time interval in Master conditions will not shorten the report generation. Currently only working for 1 second but variation possibility will be provided.

Change the naming convention of the experiment unit. ‘pump-red’ will become ‘red-pump’

Scale and decimal points of x axis.

Roadmap

Process flow diagram

Sorting of the graph in the report

Graph data export in CSV or xlsx or json format.

Support

Add another configuration as required (e.g. configuration with system voltage as input, configuration with water input to cold tank, configuration with 2 wash tank)

Last updated: 5 July 2021