ITHACA® DYNAMIC CHEMICAL PROCESS SIMULATOR

Quick Start Guide

June 2018

ITHACA® Dynamic Chemical Process Simulator

Quick Start Guide

Document Control

Document No.	Issue Date
EPT-M-010103-02-0	13/05/2018
EPT-M-010103-02-1	7/06/2018

Copyright

Disclaimer

The exercises presented herein have been designed to convey ITHACA concepts and features, and as such employ simple examples for illustrative purposes only. These examples may not be suitable for an industrial application without additional research and validation by the user.

Trademarks

Element Process Technology
support@elementprotech.com
+61 7 3106 8967
elementprotech.com
Brisbane, Australia

Table of Contents

1 Introduction

ITHACA is a combined continuous-integration and event-driven chemical process simulator. Users create and configure a network of nodes in which each node is a volume capable of material mixing, chemistry and energy transfer. Each link between nodes is one of a variety of types that manage material and data flow. Monitoring and control elements such as charts, calculators, timers, stochastic value generators and PID controllers are added to build rich, robust flowsheets that can be used to predict the behaviour of complex real-world processes over time.

Models of real-world unit operations are built by combining one or more of the basic elements described above. Once complete, the models can be saved to a library as single objects. Almost any type of unit operation can be modelled to at least project-level fidelity.

Information output from the simulator is via Excel files containing time-series process data. Each row of data represents the state of the simulated process at the specified time.

2 Overview

This guide takes the user through three exercises that cover most features of ITHACA, and expands on the principle of building unit operation models from basic building blocks. Features not covered here, such as Monte Carlo simulation and energy balancing, are covered by the User Manual.

These exercises have been designed to convey ITHACA concepts and features, and as such employ simple examples for illustrative purposes only. These examples may not be suitable for an industrial application without additional research and validation by the user.

3 Getting Ready

3.1 Install

To install the software decompress the .zip file downloaded from elementprotech.com, double-click the setup file (Setup.exe) and follow the prompts. Running Setup.exe will install the ITHACA application as well create the directory *C:\Users\Public\Documents\Public Documents\ITHACA*, inside which the following files are saved:

- The User Manual
- This document
- A selection of equipment icons that can be used to improve the visual appearance of flowsheets
- A selection of ITHACA demonstration models
- A library of example equipment models

Any new installation will first require removal of an existing installation if one is found. Multiple versions of ITHACA can, however, remain installed on a single machine if the install folder name of an existing installation is manually changed to something other than 'ITHACA', for example 'ITHACA *[old version number]*'.

Please contact support@elementprotech.com if assistance is required during installation.

3.2 Run

ITHACA can be launched by clicking the ⬤ shortcut icon in the Start menu or by double-clicking any .ith file. Copying the shortcut icon onto the quick-access bar will allow ITHACA to be conveniently launched from this location also.

On launch a splash screen is displayed which indicates the software version number and user subscription information.

4   Exercise 1 – Single Stage Chemical Reactor

This exercise steps through the creation of a continuous stirred tank reactor (CSTR), with chemical reaction between chlorine gas and sodium hydroxide solution. The energy balance will not be simulated for this exercise.

4.1   Get Started

1. Create a folder in a convenient location on your computer, for holding Exercise files. This folder will be referred to as the exercise folder in later steps
2. On start-up of ITHACA the initial view is of the MODEL pallet of tools above a set of two flowsheet sections. In the Options block of tools change the units selection to **t, m^3, kgmol, MJ**
3. Click **File**>**Save**, or alternatively click the 💾 button. Supply a filename and save into the exercise folder

4.2   Add Components

1. Click **Components** at top left of screen to open the Component Database Manager
2. Click **Create New Database**. Supply a file name and save it in the exercise folder.
3. Click **Add Phase**
4. Select the newly added phase in the tree node diagram by clicking the node text. Do not check the checkbox yet. The Phase Properties input fields will now be enabled.
5. In Phase Properties, select Liquid state
6. Enter an optional descriptor, for example 'Aqueous'
7. Leave the mixture model as Aggregate
8. Select the phase in the tree node diagram to apply these inputs. The **Add Component** button will now be enabled
9. Click **Add Component**. This will add a blank component to the selected phase.
10. Select the newly added component tree node; Component Properties input fields will now be enabled
11. In Component Properties, add a water component:
    a. Type 'Water' into the Name field
    b. Type 'H2O' into the Chemical Formula field
12. Repeat steps 8-11 to add the remaining liquid phase components as per the following data:

Name	Chemical Formula	Density
Sodium Chloride	NaCl	2.165
Sodium Hydroxide	NaOH	2.13
Sodium Hypochlorite	NaClO	2.49

13. Add an additional phase with the following properties:

State	Descriptor
Gas	Ideal

14. Add two components to the new phase with the following data:

Name	Chemical Formula
Inert	N2
Chlorine	Cl2

15. Check all phase and component checkboxes in the node tree. This adds the checked items to the model, as indicated in the right-hand side node tree.
16. Click **OK**

4.3   Add and Configure a Process Unit and Streams

1. Add an ITHACA process unit (IPU) by selecting **Unit Operations**>**Add ITHACA Process Unit** from the tools pallet at top left of screen. Alternatively, right click anywhere on the Section 1 page and select **Add IPU**
2. Left double-click the IPU to open its menu
3. Change **Overflow Volume** to 20 m^3
4. Select the **Initial Condition** tab and enter the following data in the **Components** panel:
   - Water (H2O) (t): 20
5. Click the gas phase row in the **Phases** panel to change the **Components** view to the gas-phase components
6. Add some Inert gas mass (for example 0.1 t)
7. Click **Pressurise to Op. Pressure**. This adjusts gas phase mass to achieve the specified operating pressure of the IPU, currently at the default value of 101.3 kPa, while maintaining gas component concentrations.
8. Select the **Chemistry** tab and click **Add**
9. Add the following chemical reaction:

   1 Cl2(g) + 2 NaOH(l) —> 1 NaCl(l) + 1 NaClO(l) + 1 H2O(l)

   with the following procedure:

   - Select the Chlorine node on the node tree and click **+R**
   - Select Sodium Hydroxide on the node tree and click **+R**
   - Select Sodium Chloride on the node tree and click **+P**
   - Select Sodium Hypochlorite on the node tree and click **+P**
   - Select Water on the node tree and click **+P**
   - Click **Auto Balance** to adjust stoichiometric quantities
10. From the radio buttons select the **Rate of disappearance...** option and check the **Liquid** and **Gas** checkboxes.

11. Copy the following expression into the **Reaction Rate** input field:

$$1.5*10\textasciicircum-2*UCCP(0,6,-3,5)*UCCP(0,3,-2,5)$$

The function UCCP retrieves the concentration of a component in specified phases, in specified units

> 💡 *Clicking **f(x)** in the MODEL menu pallet will open a user function quick reference guide that summarises the available functions and their syntax and usage.*

12. Click **OK** on this window and the next. IPU setup is complete
13. Save the model

4.4   Add and Configure Streams

The IPU's stream and datalink attachment ports are illustrated below for reference:
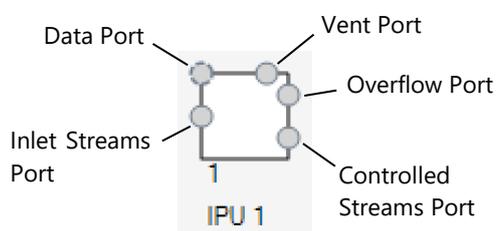
1. Right-click to the left of the IPU and select **Add Source**
2. Click the left mouse button down on the Source element and hold it down while dragging the pointer to the input port on the IPU, then let the mouse button go. A stream will be created
3. The type of stream just created is a Controlled stream, which means that its behaviour is completely specified by user input. Double-click the stream to open its window
4. Change its **Description** to Flue Gas
5. Select the **Composition** tab
6. Set gas phase concentration to 1 w/w. Note that the component panel display changed to show gas phase components when the gas phase was clicked
7. Set Chlorine concentration to 0.2 w/w
8. Select the **Flow Control** tab
9. Enter 1 (t/h) in the **Flowrate Expression** input field
10. Click **OK**
11. Add a second input stream and open its window
12. Specify input parameters as follows:
    a. Description: Fresh Scrub Liquor
    b. Phase composition: 1 w/w liquid
    c. Liquid composition: 10 g/L Sodium Hydroxide
    d. Flowrate: 100 t/h
13. Add a Sink by right-clicking above and to the right of the IUP and selecting **Add Sink**
14. Draw a stream from the IPU's vent port to the Sink
15. The stream added is a Vent stream, which controls gas pressure so as to not exceed the IPU's specified operating pressure

16. Add another Sink to the right of the IPU and draw a stream from the IPU's overflow port to the new Sink
17. The stream added is an Overflow stream, which controls combined solid and liquid volume so as to not exceed the IPU's specified overflow volume
18. Add a graph to the flowsheet by right-clicking anywhere on the section and selecting **Add Graph**
19. Activate the Graph input fields by left-clicking it once, then in the graph description field enter 'Vent Cl2 (t/h)'. The Graph input fields are disabled when the mouse pointer leaves the Graph area
20. In the graph expression field enter 'SMC(3,6)'. The aim is to plot the mass flow of chlorine gas in the vent stream. If the number of your vent stream is not 3, use your vent stream number in the expression instead
21. Add a second Graph with description 'IPU Cl (g/L)' and expression 'UCEP(1,17,-2,2)'. This will plot the concentration of chlorine in the process unit liquid phase, in units of grams per litre
22. Save the model

4.5 Simulate

1. Click the **SIMULATE** button at top left of screen
2. Set a simulation length of 4 hours in the menu bar at top of screen
3. Click the ⏺ (run) button to run a simulation. Simulation data is output in Excel format once simulation is complete
4. Become familiar with the data output file. All fundamental process data is output so that more complex parameters, such as concentration, can be calculated. The following figure plots IPU 1 liquor concentrations from this exercise as an example:
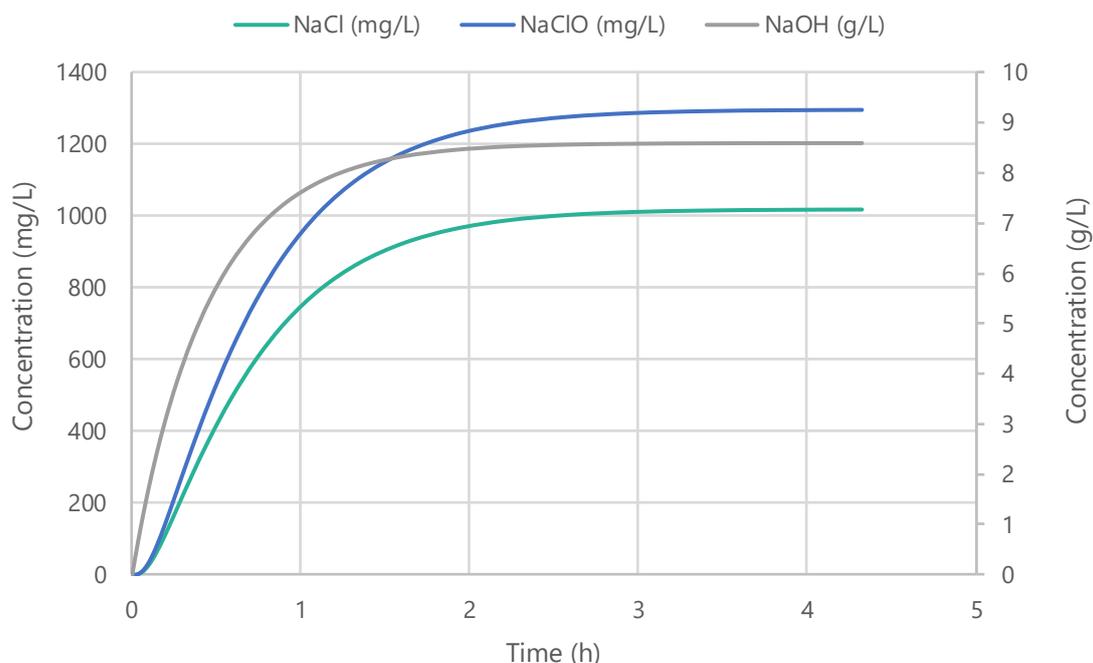
5 Exercise 2 – Multi-Stage Gas Scrubber

This exercise steps through the creation of a more complex equipment model, building on the work completed in Exercise 1 to build a scrubber model with multiple equilibrium stages.

5.1 Getting Started

1. Open the ITHACA file created in Exercise 1. This can be done through the application by clicking **File**>**Open** and navigating to your folder, or simply by double-clicking the file (.ith) outside the application.
2. Save the file with a new file name in the exercise folder. Because a copy is being generated by the application the new model file remains linked to the component database.

5.2 Add and Configure Process Units

1. Add an Expression element to the flowsheet by right-clicking on the flowsheet near the IPU and selecting **Add Expression**
2. Open the Expression editing window by double-clicking it
3. Replace the '0' expression with '1.5*10^-2' and change its description to 'Rate Constant (1/M.s)'. Click **OK**
4. Rename the existing IPU to 'Stage 1'
5. Open the reaction editing window for the chemical reaction in Stage 1, and in the Reaction Rate input field replace '1.5*10^-2' with 'EO(-1)'. This constitutes the first part of the link to the reaction rate constant value held by the Expression element. Close the reaction and IPU editors
6. Select the IPU by left-clicking it once, then right-click it and select **Duplicate**>**5 Times**
7. For this exercise we will model the scrubber with 5 equilibrium stages – currently there are 6. Select one of the IPUs, right-click it, select **Delete** and confirm the operation
8. Rename the new process units 'Stage 2',... 'Stage 5'
9. Connect the Stage 1 vent stream to the Stage 2 inlet port as follows:
    a. Holding the shift key, left-click the vent stream and then left-click the Stage 2 inlet port. Let go of the shift key
    b. Right-click any of the selected items and select **Change Stream Destination**
10. Draw vent streams connecting Stage 2 to Stage 3, Stage 3 to 4 and Stage 4 to 5
11. Draw a vent stream connecting Stage 5 to a Sink
12. Change the input Fresh Scrub Liquor stream destination to Stage 5
13. Connect an overflow stream from Stage 5 to Stage 4, Stage 4 to 3, Stage 3 to 2 and Stage 2 to 1. Be aware that other streams may need to be moved out of the way to enable the addition of new streams
14. Draw a link from the Expression element to the dataport of each IPU. This completes the linking of the Expression element to each IPU's reaction rate
15. To reduce clutter, go to **Flowsheet** in the menu bar and select **Show/Hide Data Ports**. Your flowsheet should now look something like this:
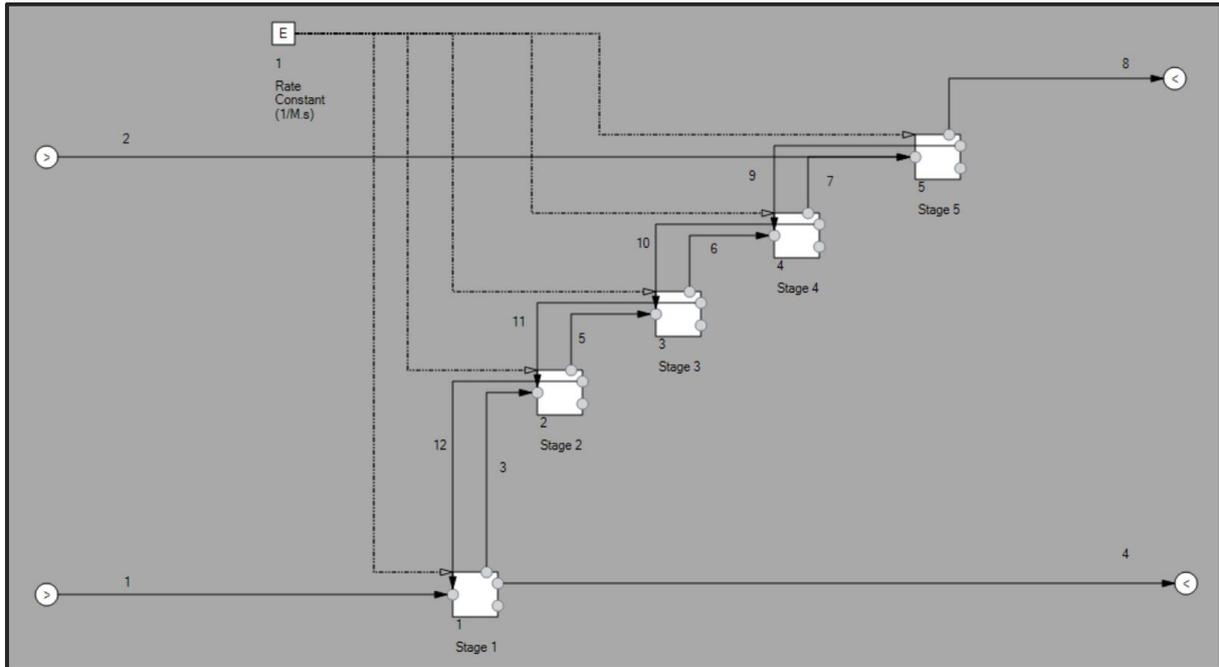
5.3   Improve the Visuals

1. Rename the following streams. The stream numbers below relate to the streams in the figure above. If stream numbers are different in your flowsheet, select the equivalent process stream:

| Stream	Description
1	Flue Gas Inlet
2	Scrub Solution Inlet
4	Scrub Solution Outlet
8	Clean Gas Outlet

2. Select all elements of the flowsheet except the Source and Sink elements. Do this by holding down the left mouse button and dragging a selection square to encompass the required elements
3. Right-click one of the selected elements and select **Group**. The selected elements are now wrapped into a single Group object represented by a single node
4. Double-click the Group node and change its name to 'Chemical Scrubber'. Note that the Expression element that has been included in the Group now appears as an input in the Group editor window

> 💡 *Complex Grouped unit operation models may be created by a specialist and used by non-specialists. In this case, creating a custom menu for a Grouped model is a good way of allowing non-specialist users to interact with and configure it without needing to understand or navigate the model's underlying logic.*
>
> *Expression elements are used for this purpose: whenever an Expression element is included in a Group, its label and input field become elements of that Group's menu. The menu is opened by double-clicking the Group icon.*

5. Move the name tag out of the way, select the Group node and right-click. Select **Replace Icon** and navigate to the Equipment Icons folder that was loaded into the Public Documents folder as part of the ITHACA installation. On standard Windows machines this will be located at *C:\Users\Public\Documents\ITHACA\Equipment Icons*. Select an image from this folder. Alternatively, select an image of your choice from any other location

6. Select and right-click the new image and select **Lock/Unlock Ports**. Port outlines change colour to blue indicating that they are now moveable

7. Drag each port to the desired location on the equipment image. Note that the tool-tip of each port reflects the name of its connecting stream

8. Select Lock/Unlock Ports again when port locations are finalised

9. Change the expression in the Vent Cl2 (t/h) Graph to reference the Clean Gas Outlet stream by changing the stream ID argument to the appropriate integer value. Graphs can be enlarged by holding and dragging their bottom-right corners. The Data Source panel of each Graph can be hidden (and shown) by clicking once on the chart panel

10. Tidy up streams as desired. The flowsheet should now look similar to the following figure:
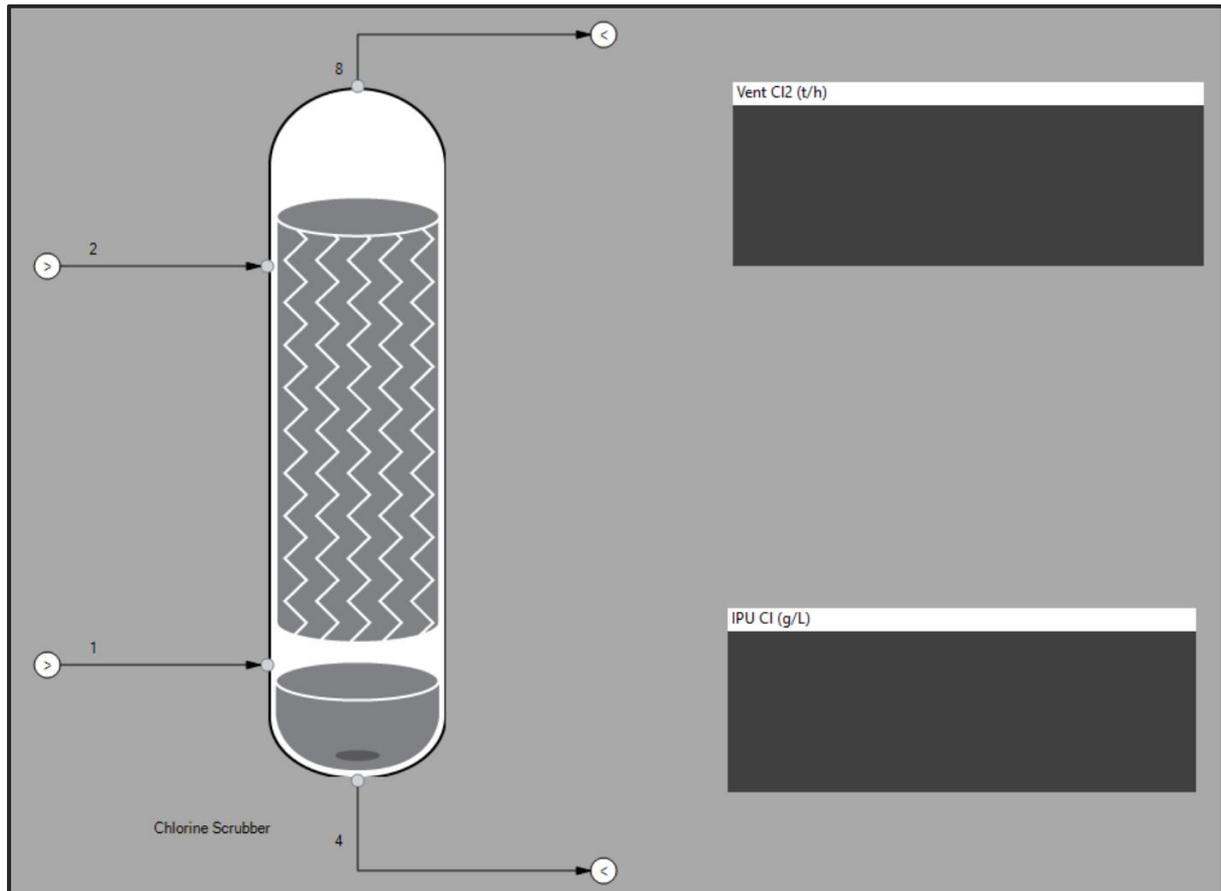
5.4 Simulate

1. In the SIMULATE menu pallet set a simulation length of 4 hours and run a simulation
2. Selected component flow-rates from output data is plotted below for comparison
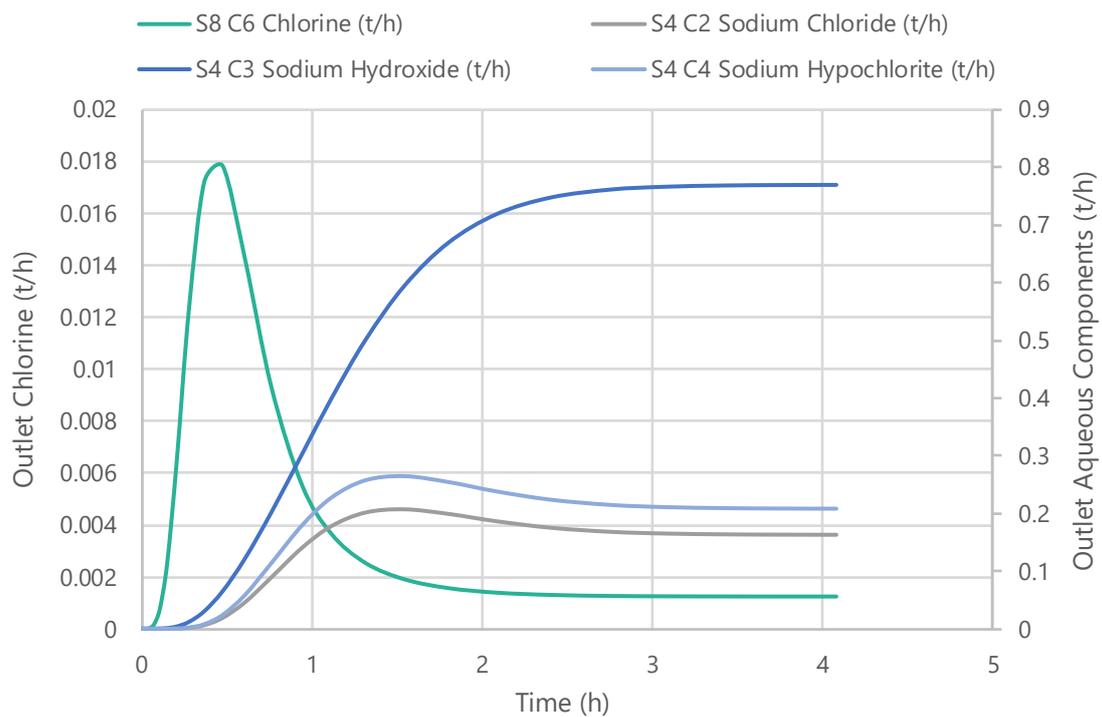
3. Double the reaction rate constant for all stages (from 1.5*10^-2 to 3.0*10^-2)
4. Run another simulation and observe the effects of the faster reaction rate

5.5 Store the Model

To make the Chlorine Scrubber model available for duplication and reuse in other flowsheets we will now store it in a library:

1. Click **Customisation>Libraries** in the **MODEL** menu bar. The libraries manager will open at right of screen
2. In the libraries manager click **Create New** and specify a location and file name. The library just created will also be opened in the manager and will appear in the Libraries list
3. Select the newly created library in the Libraries list. The contents of this library (currently zero) are now shown in the library contents panel
4. Select and right-click the Chlorine Scrubber model on the flowsheet. Select **Add to Library** from the context menu. The model will be listed in the library contents panel
5. The model has now been stored. Close the libraries manager by clicking **Close** at top right

6 Exercise 3 – Multi-Unit Scrubbing Flowsheet

This exercise steps through the creation of a flowsheet consisting of more than one equipment item, using the Chlorine Scrubber unit developed in Exercise 2. The flowsheet will simulate the start-up of the scrubbing column in closed circuit with a scrub solution tank while fed a time-varying flue gas.

6.1 Getting Started

1. Start the application and save a new model (blank flowsheet) in the exercise folder, with a name of your choice.
2. This model is not yet linked to a component database; we will link it to the database created in Exercise 1. Open the Component Database Manager and click **Switch Database**; select your Exercise database
3. Add phases and components from the database into this model by checking the check boxes. In this case all of the phases and components are required

> 💡 *The separation of components in the database from components in models allows for a single large, enterprise-wide database of components to be developed over time, with only selected components brought across into individual models as required.*

6.2 Add and Configure Process Units

1. Open the Libraries Manager. Inside the Manager, open the library created in Exercise 2
2. Select the library in the Libraries panel
3. Select the Chlorine Scrubber in the Library Contents panel, then click **Add.** Drag the model to roughly centre of screen

> 💡 *Data transfer links between flowsheet elements can be made either by referencing an element ID or drawing a datalink. The ID reference method is generally preferred since this minimises flowsheet clutter and is slightly faster during simulation; however, the user of datalinks is essential when a model will be sent to a library and re-used in other flowsheets since element IDs are almost certain to be different and will no longer match ID references.*

4. Select the column just added and right-click. Select Open Menu then Stage 1 from the drop-down menu. Note that IPUs add from the Library contain zero components
5. Fill Stage 1 with inert gas and click **OK**
6. Right-click the column again and select **Copy Properties of…**, then select Stage 1
7. Right-click again and select **Paste Properties to…** and left-click Stages 1 to 5, the **CLOSE**. Note the change of colour of items to which properties have been pasted
8. Add an IPU to the right side of the scrubber. Resize this to have an overflow volume of 100 m^3 and a total volume of 110 m^3. Fill the IPU with 10 g/L NaOH solution and rename it to 'Scrub Solution Tank'

6.3 Add and Configure Streams

1. To the Scrub Solution Tank:
   a. Add an input stream supplying water at 100 t/h

b. Add another input stream supplying 100% NaOH; this stream will control caustic concentration in the tank. In the Flow Control tab select **PID** and enter the following data:

KP	0.5
KI	0.1
KD	0
PV	UCCP(*[IPU ID]*,*[NaOH component ID]*,-2,2)
SP	10
Action	Reverse

    c. Add an overflow stream terminating at a sink

    d. Add a controlled stream terminating at the scrub solution inlet of the scrubbing column. Set flowrate to 100 t/h

2. Connect a stream from the column scrub solution outlet to the Scrub Solution Tank
3. Connect a stream from the column clean gas outlet to a sink
4. Add a Combiner element to the left of the column. To the Combiner add two inlet streams, each originating from a Source element; and an outlet stream terminating at the column gas inlet port
5. We will now develop a variable flue gas composition. Add two Expression elements and one Timer element to the flowsheet
6. Open one of the Expression elements and name it 'Cl Gas Conc, Unbounded'. Select the **Stochastic** radio button and go to the **Stochastic Setup** tab. Select the Inverse Gamma probability distribution from the dropdown menu and apply values of 6 and 1 for **Shape** and **Scale**, respectively. Click **OK**

💡 *Expression elements can be used to generate either directly calculated or probabilistically sampled (stochastic) values.*

7. Open the second Expression element and name it 'Cl Gas Conc, Bounded'. Since the probability distribution selected above can generate values greater than 1, we now need to bound it for use as a weight fraction input value. Enter the following expression into the Deterministic Setup expression input field: 'MIN(EO(*[ID]*),1)', where *[ID]* is the ID number of the 'Cl Gas Conc, Unbounded' Expression element. Click **OK**
8. Open the Timer element and enter the value '10' in the **Countdown Time**, **Minutes** input field.
9. Click the **Add Action** button, select the new action in the actions list and add the following text to the action input field: 'ESAMPLE(*[ID]*)', where *[ID]* is the ID number of the 'Cl Gas Conc, Unbounded' Expression element. The Timer will now cause the probability distribution to be resampled every 10 minutes of simulation time. Click **OK**

💡 *An Expression element set to output stochastic values will only change its output when its probability density function is resampled via the ESAMPLE() function.*

10. Select one of the Combiner inlet streams and name it 'Chlorine Gas Flow'. Set its composition to 100% chlorine gas

11. We do not want any gas flow through the column until the column is thoroughly wetted with flowing scrub solution, so initiation of gas flow must be delayed. Click the Modes button and expand the Flow Control property node

12. Select the Modes node and click Add Mode

13. Expand the Mode 2 node and select the Values node. Enter 'EO([ID])' in the Direct Flowrate Expression input field, where *[ID]* is the ID number of the 'Cl Gas Conc, Bounded' Expression element

14. Open the remaining input stream and name it 'Inert Gas Flow'. Set its composition to 100% inert gas

15. This stream will control the flowrate mode change event. Click the Modes button and add a second Mode to the flowrate property

16. Select the Mode 2 Values node and input '1-SMT(*[ID]*)' in the Direct Flowrate Expression input field, where *[ID]* is the ID number of the Chlorine Gas Flow stream. This will ensure that total flue gas flow is at all times 1 t/h while allowing chlorine gas concentration to fluctuate

17. Select the Mode 1 Values node. Note that the default flowrate is zero

18. Expand the Change Conditions node and select IF Condition 1. Enter '2' into the **To-Mode ID** input field and click **Add Sub-Condition** and **Add Additional Action** once each

19. Select Sub-Condition 1 and enter the following data:

Process Value Expression	TIME()
Comparison Operator	>=
Target Value Expression	1
Connection to Next	OR

This configuration will cause the flowrate property of this stream to switch from Mode 1 to Mode 2 when simulation time reaches 1 hour

20. Select Additional Action 1 and enter 'SCHANGE([ID],1,2)' in the Action input field, where *[ID]* is the ID number of the 'Chlorine Gas Flow' stream. This will cause the flowrate property of that stream to be changed from Mode 1 to Mode 2 at the same time

💡 *Flowsheet property mode change events are configured in IPUs, Controlled Streams and Action elements. By default all properties start a simulation in Mode 1.*

21. Close the modes menu and click **OK** in the stream menu

6.4 Add Monitoring Charts

1. Add three Graph elements to the flowsheet and configure as follows, supplying the correct ID numbers where required:

Graph	Description	Data Source Expression
1	Clean Off-Gas Cl (mg/m3)	SCEP(*[stream ID]*,17,-3,2)*1000000
2	Scrub Solution Tank NaOH (g/L)	UCCP(*[IPU ID]*,*[NaOH ID]*,-2,2)
3	Scrub Solution Tank Cl (g/L)	UCEP(*[IPU ID]*,17,-2,2)

2. The flowsheet should now look something like this:
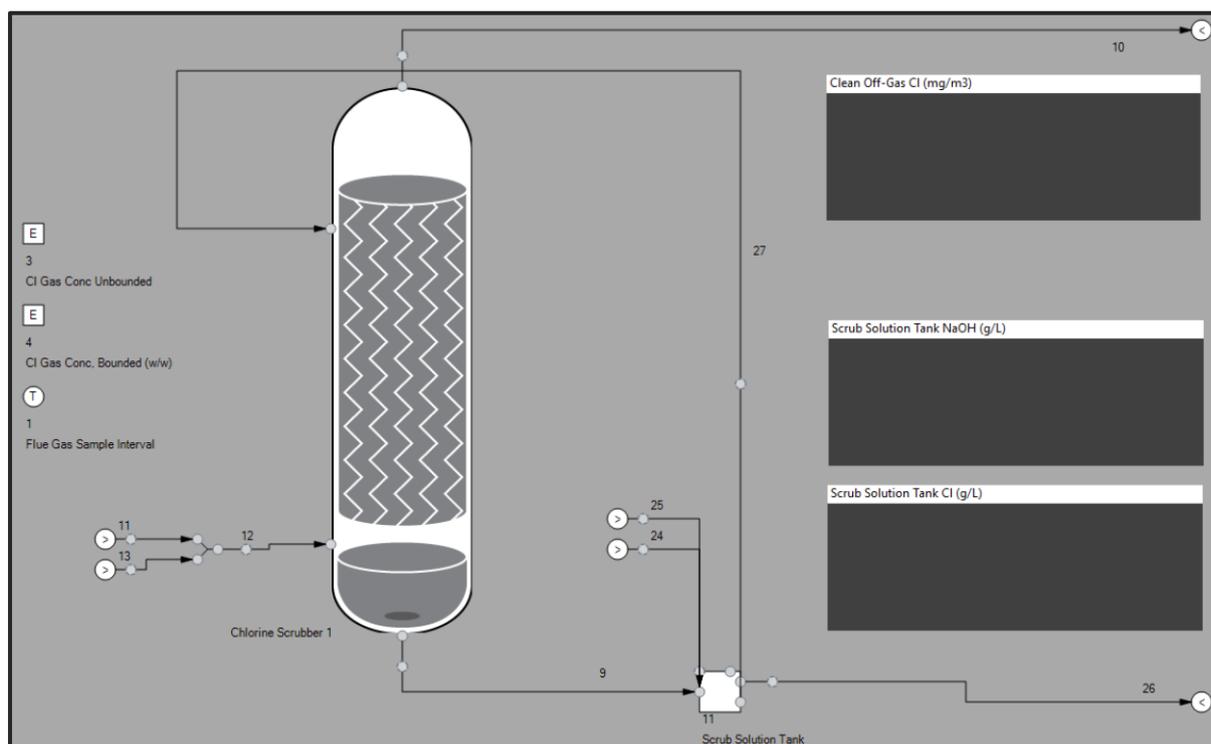
6.5 Simulate

1. Input a simulation duration of around 10 hours and click the run button
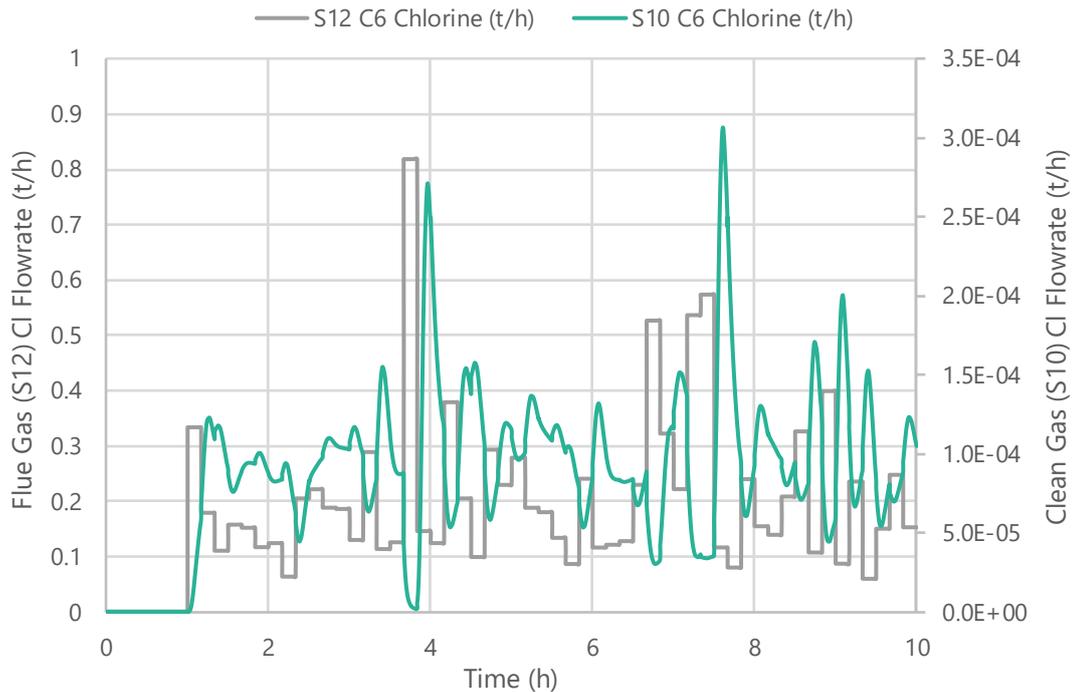2. Note that an information message appears. Click **OK**

> 💡 *If a flowsheet contains IPUs missing overflow and/or vent streams, and that flowsheet also contains overflowing or gaseous phases, then warnings will show prior to simulation since there is a possibility that overflow volume or gas pressure will be uncontrolled in one or more IPUs. These warnings can be ignored if the flowsheet configuration is such that these scenarios will not occur.*

3. Note a slight pause in simulation as events occur: column stage IPUs overflowing, probability distribution resampling and, at the 1-hour mark, a change of flowrate mode in the two flue gas component input streams

4. Click the Error and View Solver buttons to be shown live cumulative global mass error and key solver parameters, respectively.
5. Double-click streams and IPUs to open live charts plotting phase and component data. Be aware that data plotting can slow down simulation performance
6. Flue gas and clean gas chlorine flows are plotted below for comparison with your data. The input chlorine flowrate profile will be different each time the simulation is run since this is generated by the stochastic Expression element. Note the 10-minute long steps of chlorine gas input flow