ITHACA® Dynamic Chemical Process Simulator
Software User Manual

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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

The fastest and most rewarding way to learn ITHACA is to complete the exercises in the Quick Start Guide and then treat this User Manual as a reference to fill any blanks in knowledge while working on your own projects.

Example flowsheets included in the installation of ITHACA are also a good source of instruction on how to solve a variety of modelling problems.

If anything in this manual is unclear or other assistance is required, please contact us at support@elementprotech.com.

3 Installation

ITHACA is a 32-bit application designed to operating in a Microsoft Windows operating system.

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 following directory: C:\Users\Public\Documents\Public Documents\ITHACA, inside which the following useful files are saved:

- The user manual
- A quick start guide
- A selection of equipment icons that can be used to improve the visual appearance of flowsheets
- A selection of ITHACA demonstration models
- An example library of some basic unit operation 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.
4 Launching

ITHACA can be launched by clicking its shortcut icon in the Start menu or by double-clicking any .ith file. Copying the Start menu shortcut 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, the user’s subscription status and, if within a trial period or if a subscription has been purchased, also the registered user details.

5 Version Numbering

ITHACA version numbering follows a Major.Minor.Hotfix convention as follows:

- Major: any change to the software on the main development path that makes it incompatible with earlier-version code components; makes it incompatible with earlier-version flowsheet files (.ith) without manual user intervention; or significantly alters the user experience and/or established workflows. Incrementing this value resets Minor and Hotfix values to zero.
- Minor: any change to the software on the main development path, whether feature addition, feature improvement or bug fix that is not a Major change. Incrementing this value resets the Hotfix value to zero.
- Hotfix: any change to a released version of the software, generally limited to bug fixes. Any hotfixes are also incorporated into the code on the main development path.

6 Terminology

Throughout this manual the terms ‘phase’, ‘component’, ‘model’, ‘flowsheet’, ‘simulate’ and ‘simulation’ will be used regularly. These terms are to be understood as follows:

6.1 Component

**Noun**

Refers to a class of material that will be tracked during simulation. These are user-defined and often equate to chemical species; however, they may also be defined, for example, as unprocessed rock other bulk material without any specified chemical formula. Each component must be a member of a phase.

Usage example: *The user defined a component called ‘Water’ and assigned it appropriate chemical and thermodynamic properties.*
6.2 Phase

**Noun**

Refers to a class of components linked by having similar bulk properties. Each phase comprises components which collectively characterise that phase.

Usage example: *The user defined and aqueous phase that contained water, sulphuric acid and sodium sulphate components.*

6.3 Model

**Noun**

The total of the building blocks and input data that constitute a logical unit within a flowsheet.

Usage example: *Both the reactor and rainfall models predated the latest changes.*

**Verb**

The act of building a model.

Usage example: *To build a reactor model first right-click...*

6.4 Equipment Model

**Noun**

A model of a real or imagined piece of physical plant, as in reactor model.

Usage example: *The user developed two reactor equipment models: a simple model for high-level project simulations and a complex model for high-fidelity simulations with a smaller focus.*

6.5 Flowsheet

**Noun**

The total of all equipment models within one .ith file. Generally these are interlinked and operate as a whole during simulation. The name originates from the large sheets of paper on which are printed: the unit processes, directions of material flow and control logic of a real process plant.

Usage example: *The flowsheet was complex, containing many recycle streams.*

6.6 Simulate

**Verb**

To solve the material and energy balance equations for a model flowsheet at each step through time until the desired endpoint is reached. At each step the user-defined control and input logic is implemented and events fired as required. The output is a set of data tables detailing the state of the flowsheet at each time-step.

Usage example: *To simulate click Run.*
6.7 Simulation

Noun
The sum total of events and outputs that constitute the simulating of a flowsheet.
Usage example: *The simulation confirmed the suspicions of the design team*...

Verb
The act of simulating a flowsheet.
Usage example: *Simulation of the flowsheet confirmed the suspicions of the design team*...

7 Typical Workflow

7.1 Model

Specify Components
If starting a modelling project from scratch the workflow will usually begin with defining the components that will be tracked throughout a model. Component physical, chemical and thermodynamic properties are given values and the resulting component database is saved for reuse and sharing.

If the component database needed for a modelling project already exists then this can be reused.

Build Flowsheet
The basic ITHACA building blocks are connected and configured in such a way that the resulting flowsheet will, when simulated, provide the data required for the project.
Any models that are likely to be used again can be saved to one or more libraries.

7.2 Simulate
The state of the flowsheet is stepped through time from its specified initial state to its final state, via all intermediate states incorporating discrete events as well as time-varying inputs, chemistry, phase changes and controller states.
At the completion of simulation, data tables are output to an Excel file.

8 File Management

8.1 Model
Model files consist of a central .ith file which contains all ITHACA object data, and an .ifl file for each flowsheet section in the model.

8.2 Component Database
Phase and component data is stored in .idb files. A model is linked to a component database via the software user interface.
8.3 Simulation Results
When a model is simulated for the first time a results folder is generated in the same location as the .ith file and result data files are saved into it automatically. Subsequent simulation data output is also saved here.

8.4 Libraries
Libraries are independent files with an .iml extension. Libraries are created and accessed via the software user interface.

8.5 Equipment Icons
During installation of ITHACA a package of equipment icons is saved to the following location: C:\Users\Public\Documents\Public Documents\ITHACA Equipment Icons.
9 Component Definition

Phases and components are specified in the **Phases and Components** screen, accessed by clicking **Components** in the menu bar of the **MODEL** screen. The node tree on the left side displays the phases and components present in the database. The node tree on the right displays those phases and components that have been added to the currently open model. The centre area of the screen displays property values of the currently selected phase or component, as entered by the user. An example is illustrated in the following figure:

*Figure 1: IPU Equipment Parameters Editing Window*
9.1 **Switch to an Existing Database**

An existing database (.idb file) can be linked by clicking the **Switch Database** button and selecting the file. Doing so will remove any components already added to the currently open model.

9.2 **Create New Database**

A new database is created by clicking the **New Database** button and supplying a file name and location in the **Save File** dialogue. Any required phases and components will need to be specified.

9.3 **Add Phase**

To add a phase select the Database node text and click **Add Phase**.

9.4 **Remove Phase**

To remove a phase select its node text and click **Remove Phase**.

9.5 **Add Component**

To add a component select its intended parent phase node text and click **Add Component**.

9.6 **Remove Component**

To remove a component select its node text and click **Remove Component**.

9.7 **Adding Phases and Components to a Model**

To add phases and components from the database into the currently open model, check their respective checkboxes. The order of addition of components can be important. It is recommended that the first component within each phase added to the model is a component that generally constitutes a large portion of the phase, for example water for an aqueous phase.

9.8 **Specify Phase Property Values**

To specify phase property values select its node text and enter appropriate data. The entry of data into the **Descriptor** field is optional and can be used to further classify the phase type. This value will appear in parenthesis next to its state when appearing in lists, for example **Solid (Inorganic)**.

**Mixture Model**

When the phase state is Liquid the mixture model can be set to either Aggregate or Solution, which determines how phase density is calculated. Density of an Aggregate liquid is calculated as the mass-weighted average of the density of each pure constituent component. Density of a Solution liquid is calculated as the mass-weighted average of the density of each component as defined by each component’s concentration-density equation.

Use of the Solution mixture model is slightly more computationally intensive during simulation than use of the Aggregate model.
9.9 Specifying Component Property Values

To specify a component’s property values select its node text and enter appropriate data.

**Phase Member Type**

Phase Member Type applies only to components in a Liquid phase using a Solution mixture model. Options are Solvent and Solute. Each Liquid Solution phase must have one Solvent component.

**Chemical Formula**

A chemical formula is required only if the component is intended to be used in chemical reactions. Formulae can be entered if required, for example $A$ and $B$ could be used to represent fictional substances. A chemical reaction $A \rightarrow B$ could subsequently be defined in process units. Entering the formula of a real chemical will trigger calculation of the component’s molar mass. If, however, for example $B$ was entered as the chemical formula but it was not intended to represent the element boron then the calculated molar mass can be overwritten as required.

**Density**

Components in an Aggregate phase require an estimate of the density of the pure component. Where real-world solution components are concerned the density of the pure anhydrous solid may provide a reasonable value for pure component density in solution.

A Solvent component in a Solution Liquid phase requires only a pure component density. For example a density of 1 kg/L could be provided for water.

A Solute component in a Solution Liquid phase requires at least 3 non-zero concentration-density data pairs including the pure solvent pair. A quadratic equation is fitted to the data to provide a continuous concentration-density relationship for simulation.

**Specific Heat of Formation**

Required only if energy balancing. The heat of formation is used to calculate heats of reaction.

**Specific Heat Capacity**

Required only if energy balancing.

**Specific Heat of Solution**

Required only if energy balancing and the heat of solution is significant. The top row of data is the dilution ratio in terms of moles of solvent per mole of solute. The bottom row of data is the corresponding heat absorbed relative to the pure component. Negative heat values signify heat release. All 5 dilution ratio-heat data pairs are required and should not include the pure state (0,0) pair. The right-most data pair is assumed to represent infinite dilution.

The following model is fitted to the data to provide a continuous relationship for use in simulation:

$$
\Delta H_{\text{soln}} = \Delta H_{\text{soln}}^{\text{inf}} \times (1 - e^{c_1 r^{c_2}})
$$

where:

$r$ = dilution ratio
\[ c_1, c_2 = \text{constants} \]

**Coefficient of Volumetric Thermal Expansion**

Required only if energy balancing and thermal expansion is significant. Currently only a constant value is accepted.

**Dissociation Constant**

A positive value indicates the moles of dissociated hydrogen ions per mole of component, and a negative value indicates the moles of dissociated hydroxide ions per mole of component. Non-integer values can be used. This value is used to estimate Liquid phase pH.

## 10 Flowsheet Building Blocks

### 10.1 ITHACA Process Unit

The ITHACA Process Unit (IPU) is a constant-volume vessel in which chemistry, phase transitions, energy transfer and events can be configured. IPUs have the following properties whose values are set by the user:

- Name
- Description
- Total Volume
- Overflow Volume
- Operating Pressure
- Operating Temperature
- Input Heat
- Input Work
- Status

**Usage**

An IPU is used to model any part of a process that can be reasonably represented as a single volume. While an IPU can obviously represent a unit operation with homogeneous contents such as a well-mixed tank, it can also represent a unit operation with heterogeneous contents such as a settler or a stage of a scrubbing column due to the three types of stream that are available to withdraw material from an IPU in different ways.

In order to simulate unit operations that exhibit plug flow or pseudo-plug flow behaviour, multiple IPUs should be connected in series. The greater the number of IPUs connected in series, the closer the model behaviour will be to true plug flow, but the slower any subsequent simulation of the model will be. True plug flow is rarely if ever seen in real-world process equipment, even in pipes, since this would require frictionless equipment walls to prevent drag from forming a velocity profile that in turn causes back-mixing.
**Ports**

The IPU has five ports, as indicated in the following figure:

![Figure 2: IPU Ports](image)

- **Inlet Port**: connect any number of incoming process streams.
- **Vent Port**: connect a single vent stream to control IPU gas pressure.
- **Overflow Port**: connect a single overflow stream to control IPU non-gas material volume.
- **Controlled Port**: connect any number of Controlled streams to withdraw material at user-defined flow-rates and compositions. These streams are used in conjunction with IPUs to create physical separation models, for example thickeners, filters, solvent extraction cells, etc.
- **Data Port**: connect any number of incoming and outgoing datalinks to create information transfer links that are independent of equipment IDs between building blocks that need to reference one another.

**Menu Access**

Specifying IPU parameter values, chemical reactions and initial conditions is undertaken via the IPU menu. The menu is opened by either double-clicking an IPU icon or selecting an IPU icon and navigating to **Unit Operations->Open IPU Menu** in the menu bar of the **MODEL** screen.

**Equipment Parameters**

Equipment parameter Mode 1 values are specified in the Equipment Specification tab of the IPU menu, as illustrated below:
Value types for equipment parameters are as follows:

- **Name** – any alphanumeric string
- **Description** – any alphanumeric string
- **Total Volume** – any numeric value greater than zero
- **Overflow Volume** – any numeric value greater than zero and less than or equal to Total Volume
- **Operating Pressure** – any numeric value greater than zero
- **Operating Temperature** – any numeric value greater than -273°C
- **Input Heat** – any numeric value. Negative values are output heat.
- **Input Work** – any numeric value. Negative values are output work.
- **Status** – Select from drop-down menu. Selecting SIMULATE includes the IPU in simulation calculations. Selecting IGNORE excludes the IPU.
Chemistry

Chemical reactions are specified in the Chemistry tab of the IPU menu, as illustrated below:

*Figure 4: IPU Chemical Reactions Management Window*

Click **Add** to add a new reaction. This will open a new window for specifying details.

Select an existing reaction and click **Edit** to open a new window for editing its details. Alternatively double-click a reaction to open its editing window.

Select an existing reaction and click **Delete** to remove it from the IPU.

The reaction editing window is illustrated in the following figure:
A reaction equation is specified by selecting components from the node tree and clicking either +R to add it as a reagent or +P to add it as a product. -R and -P are used to remove selected components from the equation.

Reaction components are added with an initial stoichiometric coefficient of 1. To balance the equation click Auto Balance, or if this is for some reason unsuccessful click User Balance. A window will open allowing the user to manually enter coefficients.

Every reaction must have an associated rate at which it proceeds during simulation. This may be specified in three different ways, and is always applied relative to the leading (left-most) reagent component in the equation:

- Fractional Conversion of Incoming – a value between 0 and 1 indicating the fraction of the incoming component to convert. The rate of reaction required is calculated. This is useful, for example, when a fixed percentage of an incoming component is always converted.
• Rate of Disappearance – an explicit rate equation supplying the rate at which the leading component is disappearing in units of moles per second per litre. The phases to be included in the unit volume calculation can be specified via the Solid, Liquid and Gas tick-boxes. For example the rate of leaching of copper sulphide into solution might be specified per unit volume of slurry (solid + liquid) even though an oxidising gas is also present. When the **Allow Reverse Reaction** tick-box is ticked the reaction is allowed to proceed when the rate of disappearance is negative. There are many cases where reverse reaction is not desirable, for example a metal precipitation reaction should not proceed when solution pH is below the saturation pH for a given concentration of that metal.

• Equilibrium Value – a parameter and a target value for that parameter are supplied. The simulator then attempts to calculate the rate of reaction required to maintain the parameter on target. Note that this can only work if the parameter is initially at, or very close, to the target value.

**Initial Condition**

The initial mass of each component in an IPU is specified on the **Initial Condition** tab, as illustrated below:

*Figure 6: IPU Initial Condition Window*

Component mass and moles and phase mass and volume can be input.

**Modes**

Each equipment property and the kinetics of each chemical reaction can have multiple modes of operation. By default each has one mode – Mode 1 – this being specified via the IPU Menu fields. Mode 1 values are initially applied during simulation. There are many possible reasons for changing a property from one mode to another, for example chemical reaction kinetics may change significantly under one set of conditions versus another. Clicking the **Modes**
button opens a window that allows the addition of modes and of logic for switching between them, as illustrated below:

Figure 7: IPU Property Modes Window

Methods for switching between modes is covered in greater detail under Managing Property Modes.

Data Inputs

Clicking Data Inputs displays a list of incoming datalinks and their respective origins.

10.2 Vent Stream

A stream is a vent stream if its source port is the vent port of an IPU. The discharge end of a vent stream can connect to any input port on an IPU, Splitter, Combiner, Section Link or Sink. The vent stream Description property can be edited by the user.

Vent streams are used for control of gas pressure in the source IPU to the IPU’s specified Operating Pressure. Only gas phases will flow in vent streams.

To add a Vent Stream, left click in the Vent Port of an IPU, hold, drag to the required Input Port or other receiving object and release the mouse button.

10.3 Overflow Stream

A stream is an overflow stream if its source port is the overflow port of an IPU. The discharge end of an overflow stream can connect to any input port on an IPU, Splitter or Combiner, and any Section Off-Page Link or Sink. Overflow Streams have two user-specified properties:

- Description
- Phase selection: Solid, Liquid or both

Overflow streams are used to control solid and/or liquid volume in the source IPU to the IPU's specified Overflow Volume.

To add an Overflow Stream, left click in the Overflow Port of an IPU, hold, drag to the required Input Port or other receiving object and release the mouse button.

### 10.4 Controlled Stream

A Controlled Stream is a stream whose flowrate and composition is specified by the user. A Controlled Stream originates either at the Controlled Port of an IPU or at a Source, and terminates at any input port on an IPU, Splitter or Combiner, or any Section Off-Page Flag or Sink. Controlled Streams have the following additional properties whose values are set by the user:

- Description
- Pressure
- Temperature
- Maximum Flowrate
- Minimum Flowrate
**Controlled Stream Equipment Specification Window**

Controlled Streams are used to withdraw mass from an IPU at a user-specified rate and composition.

To add a Controlled Stream, left click in the Controlled Port of an IPU, hold, drag to the required Input Port or other receiving object and release the mouse button.

**Composition**

Controlled Stream composition may be specified in a number of ways:

- To match the total composition of a source IPU
- To match the Solid and Liquid phase composition of a source IPU
- To match the Gas phase composition of a source IPU
- Customised

Selection of these high-level options is made via the dropdown menu at bottom left of the **Fluid Composition** tab, as illustrated below. Selecting the Custom option allows the input of a user-specified composition via the input screen illustrated below. When a composition is not entered (i.e. is marked with ‘-’) then the composition of the source IPU is used.
Phase and Component compositions may be entered independently. This means, for example, that Phase composition can be controlled (for example, percent solids) without needing to specify the composition of each phase.

If a Controlled Stream originates at a Source then the user must enter a complete composition.

Figure 9: Controlled Stream Composition Window

**Flowrate**

Flowrate may be either directly specified as a constant or a function of other values, or it may be controlled by a proportional-integral-derivative (PID) controller. This selection is made via the radio buttons illustrated in the figure below.
The PID controller solves the following equation at each time step in order to arrive at an output value:

\[
CO = K_P \left( e(t) + K_I \int_{t_0}^{t_n} e(t) \, dt + K_D \frac{d\{PV\}}{dt} \right)
\]

Where:

- \(CO\) = controller output
- \(K_P\) = proportional control factor
- \(K_I\) = integral control factor
- \(K_D\) = derivative control factor
- \(e(t)\) = error = \(SP(t) - PV(t)\)
- \(SP\) = set-point
- \(PV\) = process value
- \(t\) = time
Direct and Reverse options specify whether the controller output should increase when the process value is above set-point (Direct) or decrease (Reverse).

**Modes**

Most Controlled Stream properties can have multiple modes of operation. By default each has one mode – Mode 1 – this being specified via the Controlled Stream Menu fields. Mode 1 values are applied initially during simulation. There are many possible reasons for changing a property from one mode to another, for example stream the stream flow may need to stop or restart depending on the conditions in another unit operation, such as flows from a batch unit operation. Clicking the **Modes** button opens a window that allows the addition of modes and of logic for switching between them, as illustrated below:

*Figure 11: Controlled Stream Property Modes Window*

---

**Data Inputs**

Clicking Data Inputs displays a list of incoming datalinks and their respective origins.

10.5 **Splitter**

Splitters take an input stream and split the contents into two according to a user specification. Three types of split are possible:

- **Bulk Mass split** – a single value in the range (0,1), or a function that outputs such a value, is accepted
- **Phase split** – a value in the range (0,1) is required for each Phase present in the model
- Component split – a value in the range (0,1) is required for each Component present in the model.

10.6 Combiner
Combiners take two input streams and combines them into one. No user input is required apart from the connection of the streams.

10.7 Datalink
Datalinks are dashed lines connecting ITHACA building blocks and are used for identifying data sources without the need to refer to ID numbers. This is particularly useful when creating complex equipment models that will be copied and reused, and whose constituent building block ID values will not necessarily remain the same as the original model IDs.

Figure 12: Example Use of Datalinks

A Datalink is added by left-clicking in the dataport of an IPU or Stream, or in the body of a PID Controller, Expression, Expression List or Timer, holding, dragging to the required destination dataport or object and releasing the mouse button.
10.8 Action

The Action element is used to carry out one or more actions – such as activating a Timer or changing a Controlled Stream property mode – when user-specified criteria have been met. The Action element contains Boolean logic tools for building these criteria, and controls for adding and specifying the actions to carry out. These features are the same as mode controls for IPUs and Controlled Streams, and is covered in greater detail in Section 12.

*Figure 13: Action Element Window*

10.9 PID Controller

The PID Controller is an independent controller (i.e. not attached to a Controlled Stream) for controlling a process variable to a set-point using a proportional, integral, derivative (PID) method.

*Figure 14: PID Controller Menu*
The PID controller solves the following equation in order to arrive at an output value:

\[ CO = K_P \left( e(t) + K_I \int_{t_0}^{t_n} e(t) \, dt + K_D \frac{d\{PV\}}{dt} \right) \]

Where:

- \( CO \): controller output
- \( K_P \): proportional control factor
- \( K_I \): integral control factor
- \( K_D \): derivative control factor
- \( e(t) \): error = \( SP(t) \) – \( PV(t) \)
- \( SP \): set-point
- \( PV \): process value
- \( t \): time

Direct and Reverse options specify whether the controller output should increase when the process value is above set-point (Direct) or decrease (Reverse).

The output value of the PID Controller can be referenced by other building blocks via the CO() user function. See User Functions for more details.

**10.10 Expression**

An Expression element is used to calculate a value, with two types of value available: determinate and stochastic. The Expression element value can be referenced by other building
blocks via the EO() user function. When in stochastic mode the selected probability density function is sampled once at the start of simulation. To re-sample the function at any time call ESAMPLE().

See **User Functions** for more details on these functions.

![Figure 15: Expression Window – Deterministic (Left), Stochastic (Right)](image)

An additional use for Expressions is in defining the user input fields for the custom menu of a Grouped custom model. See **Building Custom Models** for more details.

### 10.11 Expression List

An Expression List allows input of an ordered list of inline mathematical expressions or constants.
During simulation the active item of the list is evaluated and this value can be referenced by other building blocks via the LO() user function. The active item can be advanced to the next item in the list by calling the LINCREMENT() user function, and any item in the list may be set as the active item by calling LACTIVE(). For details on the usage of these function please see User Functions.

10.12 Timer

The Timer counts down from a user-specified starting time, and carries out user specified actions when it reaches zero. The Timer countdown may be set to start immediately on start of simulation, or it can be initially deactivated by setting the Countdown Time to zero. During simulation the Timer can be activated by another flowsheet element calling the TSTART(x,y) function, where x is the Timer ID and y is the required count-down time in hours.

The Timer may be set to repeat or to countdown once only.
Typically a Timer action will be to change the mode of an IPU or Controlled Stream property, for example to switch on or off the flow in a stream, or to switch on or off the chemistry in an IPU. Mode changes are made by calling the UCHANGE() and SCHANGE() user functions. Other types of action may also be carried out, for example changing the active item of an Expression List.

Actions are added by clicking **Add Action**, and removed by selecting the action and clicking **Delete**. If more than one action is specified then the order of their execution may be significant. Actions can be reordered by clicking the ▲ and ▼ buttons as required.

### 10.13 Sources

Sources supply mass and energy to the flowsheet and as such are the origin nodes of flowsheet input streams. A Source may have connected it to a single output stream. This stream will be a Controlled Stream requiring complete user definition of flowrate and composition.

### 10.14 Sinks

Sinks take mass and energy from the flowsheet, and as such are the terminating nodes of flowsheet output streams. Sinks may have multiple input streams connected to them.
10.15 Section Link Flags
Section Departure and Section Arrival flags connect streams that cross from one flowsheet section to another. To break a stream across flowsheet sections add a Section Departure Flag and link the required stream to it. Next select the Section Departure flag and either right-click it or select Flowsheet>Link From Section Departure from the Model screen menu bar. A selection menu will appear from which the Section to be linked to can be selected. Once selected a Section Arrival flag will appear on the left-hand side of that section. Connect a stream from the Section Arrival flag to its required destination and the link is complete.

10.16 Single-Variable Graphs
Single Variable Graphs plot either a trendline or a single column depicting the value of the expression entered in the Data Source field. Graph input fields are disabled when the mouse pointer leaves the Graph area in order to ensure that the user maintains control of where input focus goes on the flowsheet. To re-enable a Graph, left click it once anywhere.

![Figure 18: Single Variable Graph](image)

Colour scheme may be selected and a title entered, and the Graph can be resized by left-clicking, holding and dragging the resize icon at bottom right of the setup panel. When Graph setup is complete the graphing area may be left-clicked once to hide the setup panel, and clicked again to unhide it. To move the Graph click, hold, drag and release the left mouse button.

11 Connecting IPUs, Streams and Datalinks
Streams and Datalinks are created by left-clicking into a Port or any Controller, Timer, Source, Section Arrival, Expression or Expression List; holding the button down; dragging the mouse arrow to the required destination Port, Controller, Timer, Sink, Section Departure, Expression or Expression List and releasing the mouse button.

The nature of the source node determines the type of stream that is created.

Once created, Stream origins and destinations may be changed as long as this does not require a change of stream type. For example, a Controlled Stream may have its origin moved to the Controlled Port on a different IPU but not to on Overflow Port.

To change Stream origin or destination, select the Stream, hold the Ctrl key and select the desired new Port or item, right-click and select Change Stream Origin or Change Stream Destination, as applicable.
12 Managing Property Modes

Mode 1 values for IPU and Controlled Stream properties are created by default and can be edited via the respective menus. Adding additional modes and configuring logic for switching between them is undertaken in the Mode Management menu, accessed by clicking the Modes button at bottom left of the IPU and Controlled Stream menus.

In order to add modes and configure mode change logic for a given property, first expand out the property node to view all sub-nodes.

12.1 Add Mode

To add a mode to a property select the Modes node and click Add Mode.

12.2 Remove Mode

To remove a mode select the applicable Mode node and click Remove.

12.3 Configure Mode Change Logic

Simulation by default starts by using Mode 1 values for all properties. During simulation the flowsheet is stepped through time. After each step the simulation engine checks whether one or more events, including mode change events, have occurred (been stepped over), and if so the solution is back-tracked to the time of the earliest such event.

If Mode 1 and Mode 2 have been configured for an equipment property the time at which a mode change should occur is specified as follows:

1. In the node tree select Mode 1 IF Condition 1.
2. In the To-Mode ID field enter the ID of the mode to be change to, in this case 2.
3. Click Add Sub-Condition
4. Expand out the Sub-Conditions node and select Sub Condition 1
5. In the Process Value Expression field add an expression that returns the value of interest. This could simply be simulation time if the mode change should occur at a set time, or could be a process value such as the concentration of a component or element in a given stream or vessel.
6. In the Target Value Expression field add a value or expression.
7. In the Comparison Operator field select the appropriate operator.

For example, if Mode 1 is required to change to Mode 2 at 2 hours simulation time the Process Value Expression will be TIME(), the Target Value Expression will be 2 and the comparison operator will be >=.

Multiple conditions may be specified. For example if the active mode is required to switch from Mode 1 to Mode 2 when simulation time is 2 hours OR some component concentration falls below a required value, then the Sub Condition 1 Connection To Next selection should be OR (the default value) and a second sub condition should be added with the following inputs:

- Process Value Expression: [some expression for concentration]
- Comparison Operator: <=
- Target Value Expression: [required concentration value]
If on the other hand the active mode should switch from Mode 1 to Mode 2 when simulation time is 2 hours AND some component concentration falls below a require value then set Sub Condition 1 Connection To Next to AND. Any number and combination of AND and OR clauses can be configured in this way within an IF Condition.

In the case of a set of sub conditions connected by AND statements the time of event occurrence is assessed on the first sub condition of the set. As a result the expressions entered in the first sub condition Process Value Expression and Target Value Expression fields must be continuous functions in time. Subsequent sub conditions within the AND-connected set may be discrete and Boolean functions. For example, the active mode might be required to switch from Mode 1 to Mode 2 when some concentration reaches some value AND some other condition = TRUE.

Multiple IF conditions may be configured, each with any number of constituent OR and AND clauses as described above. IF conditions are evaluated in the order in which they appear in the node tree, and consequently their order may be important for achieving the required simulation behaviour. IF conditions can be reordered in the node tree by selecting a condition and moving it up or down with the and buttons.

### 13 Building Custom Models

A custom model comprises more than one of the basic ITHACA building blocks, for example a packed stripping column might be modelled as many IPUs connected in series in order to reproduce the plug-flow behaviour expected of the real column. Controllers, Expressions, Timers, Splitters etc. may also be used in building a custom model.

#### 13.1 Grouping

Any set of building blocks can be grouped under a single node by selecting the required items, right-clicking and selecting Group or clicking Customisation>Group in the MODEL screen menu. The purpose of grouping is primarily aesthetic, hiding the constituent building blocks behind a single node representative of the custom model. The value of cleaning up a flowsheet to show only the important parts should not be underestimated in the context of clarifying communication with colleagues and clients.

It is important to note that information links between the building blocks of a custom model should be defined with Datalinks, not ID numbers. When Grouped custom models are duplicated or used in other flowsheets the ID numbers of all underlying blocks is likely to be different from those of the original custom model. This would cause any function that referenced a model by ID number to not evaluate correctly.

#### 13.2 Replacing Node Image

The default IPU and Group nodes can be replaced with an image of your choice to better reflect the function of the underlying model and further improve clarity of communication. To replace a node first select it and then either right-click and select Replace Icon or select Customisation>Replace Icon in the MODEL screen menu, then follow the prompts to select an image file of your choice. Several equipment images are supplied with ITHACA and are located in the following location: C:\Users\Public\Documents\Public Documents\ITHACA.
13.3 Custom Model Menu

Menus for the underlying models of a grouped custom model are always accessible by selecting the custom model node, right-clicking, hovering over the Open Menu item and left-clicking the underlying model of interest.

A custom model may be constructed by a specialist user for use throughout an organisation by modellers with less knowledge of the underlying logic of the custom model. In this case the specialist modeller may find it convenient to customise the menu that opens when their custom model is double-clicked. In this way just the parameters required to integrate a custom model into a particular flowsheet can be exposed to the non-specialist user, while model details remain one further step removed.

Customising a menu is as simple as adding an Expression to the custom model for every input field required in the menu, and linking each Expression to the model requiring its value. Expression names become input field descriptors in the menu once the custom model is Grouped.

13.4 Ungrouping

Ungrouping reverses the Group operation. Select the Grouped object and either right-click and select Ungroup or select Custom Models>Ungroup from the Model menu bar.

If the model is Grouped after an Ungroup operation then any previously applied equipment image is reinstated unless the underlying model has changed significantly.

14 Equipment Model Libraries

An Equipment Model Library is a collection of model files, whether they are simple IPUs or complex Grouped models. Each Library is an independent .iml file.

The purpose of Libraries is to provide storage for pre-build equipment models for re-use in other flowsheets and by other users.

14.1 Managing Libraries

To access Library functions click Customisation>Libraries in the MODEL view menu bar.

To create a new library click Create New. To open an existing library click Open – any number of Libraries may be open at once. To close the selected Library click Close. To close the Libraries Manager click Close at top-right.

14.2 Managing Equipment Models

To view the contents of a library select it in the Libraries list. This will fill the Selected Library Contents window with a list of contained equipment models.

To add a selected Library equipment model to the current flowsheet click Add. To delete an equipment model from the Library click Delete. To rename the selected equipment model click Rename.

To add an equipment model to a library, select a library in the Manager window, then select the equipment model and either right-click and select Add To Library, or click Customisation>Add Model to Library in the MODEL view menu bar.
15 User Functions

Material, equipment and simulation property values can be accessed by calling built-in user functions. These functions are presented here and are also accessible in the software by clicking the f(x) menu item in the Model view.

Table 15-1: User Functions – ITHACA Process Unit Properties

<table>
<thead>
<tr>
<th>Categories</th>
<th>Description</th>
<th>Output Value Units</th>
<th>Syntax</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Contained Material Properties</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mass</td>
<td>Mass Total</td>
<td>(kg, t)</td>
<td>UMT(ID)</td>
</tr>
<tr>
<td></td>
<td>Mass of Phase</td>
<td>(kg, t)</td>
<td>UMP(ID, pIDs)</td>
</tr>
<tr>
<td></td>
<td>Mass of Component</td>
<td>(kg, t)</td>
<td>UMCP(ID, cID)</td>
</tr>
<tr>
<td></td>
<td>Mass of Element in Total</td>
<td>(kg, t)</td>
<td>UMET(ID, eID)</td>
</tr>
<tr>
<td></td>
<td>Mass of Element in Phase</td>
<td>(kg, t)</td>
<td>UMEP(ID, eID, pIDs)</td>
</tr>
<tr>
<td>Moles</td>
<td>Moles Total</td>
<td>(gmol, kgmol)</td>
<td>UNT(ID)</td>
</tr>
<tr>
<td></td>
<td>Moles of Phase</td>
<td>(gmol, kgmol)</td>
<td>UNP(ID, pIDs)</td>
</tr>
<tr>
<td></td>
<td>Moles of Component</td>
<td>(gmol, kgmol)</td>
<td>UNCP(ID, cID, pIDs)</td>
</tr>
<tr>
<td></td>
<td>Moles of Element in Total</td>
<td>(gmol, kgmol)</td>
<td>UNET(ID, eID)</td>
</tr>
<tr>
<td></td>
<td>Moles of Element in Phase</td>
<td>(gmol, kgmol)</td>
<td>UNEP(ID, eID, pIDs)</td>
</tr>
<tr>
<td><strong>Concentration</strong></td>
<td>Concentration of Phase in Total</td>
<td>As specified</td>
<td>UCPT(ID, pID, units)</td>
</tr>
<tr>
<td></td>
<td>Concentration of Phase in list of Phases</td>
<td>As specified</td>
<td>UCPP(ID, pIDs, units)</td>
</tr>
<tr>
<td></td>
<td>Concentration of Component in Total</td>
<td>As specified</td>
<td>UCCT(ID, cID, units)</td>
</tr>
<tr>
<td></td>
<td>Concentration of Component in list of Phases</td>
<td>As specified</td>
<td>UCCP(ID, cID, pIDs, units)</td>
</tr>
<tr>
<td></td>
<td>Concentration of Element in Total</td>
<td>As specified</td>
<td>UCET(ID, eID, units)</td>
</tr>
<tr>
<td></td>
<td>Concentration of Element in list of Phases</td>
<td>As specified</td>
<td>UCEP(ID, eID, pIDs, units)</td>
</tr>
<tr>
<td><strong>Density</strong></td>
<td>Density of Total</td>
<td>(kg/L)</td>
<td>UDT(ID)</td>
</tr>
<tr>
<td></td>
<td>Density of Phase</td>
<td>(kg/L)</td>
<td>UDP(ID, pID)</td>
</tr>
<tr>
<td><strong>Volume</strong></td>
<td>Volume Total</td>
<td>(L, m³)</td>
<td>UVT(ID)</td>
</tr>
<tr>
<td></td>
<td>Volume of Phase</td>
<td>(L, m³)</td>
<td>UVP(ID, pID)</td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td>Pressure Total</td>
<td>(°C)</td>
<td>UT(ID)</td>
</tr>
<tr>
<td></td>
<td>Partial Pressure of Gas Phase</td>
<td>(kPa)</td>
<td>UPP(ID, pID)</td>
</tr>
<tr>
<td></td>
<td>Partial Pressure of Gas Component</td>
<td>(kPa)</td>
<td>UPC(ID, cID)</td>
</tr>
<tr>
<td><strong>pH</strong></td>
<td>pH of a Phase</td>
<td></td>
<td>UHP(ID, pID)</td>
</tr>
<tr>
<td><strong>Energy</strong></td>
<td>Internal Energy</td>
<td>(kJ, MJ)</td>
<td>UU(ID)</td>
</tr>
<tr>
<td><strong>Equipment Properties</strong></td>
<td>Process unit total volume</td>
<td>(L, m³)</td>
<td>UTOTALVOL(ID)</td>
</tr>
<tr>
<td></td>
<td>Process unit overflow volume</td>
<td>(L, m³)</td>
<td>UOVERFLOWVOL(ID)</td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td>Specified temperature (when not energy balancing)</td>
<td>(°C)</td>
<td>USPECTEMP(ID)</td>
</tr>
<tr>
<td><strong>Pressure</strong></td>
<td>Specified or control pressure</td>
<td>(kPa)</td>
<td>USPEC_PRESSURE(ID)</td>
</tr>
<tr>
<td><strong>Property Modes</strong></td>
<td>Process unit specified rate of heat input</td>
<td></td>
<td>UNINPUTHEAT(ID)</td>
</tr>
<tr>
<td></td>
<td>Process unit, specified rate of work on</td>
<td></td>
<td>UIINPUTWORK(ID)</td>
</tr>
<tr>
<td></td>
<td>Unit Operation Property, command to change mode</td>
<td></td>
<td>UCHANGE(ID, propID, modeID)</td>
</tr>
<tr>
<td></td>
<td>Unit Operation Property, current mode number</td>
<td>(#)</td>
<td>UMODE(ID, propID)</td>
</tr>
</tbody>
</table>
### Table 15-2: User Functions – Stream Properties

<table>
<thead>
<tr>
<th>Categories</th>
<th>Description</th>
<th>Output Value Units</th>
<th>Syntax</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Stream Contained Material:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mass Flow</td>
<td>Mass Flow of Total</td>
<td>(kg/h, t/h)</td>
<td>SMT(ID)</td>
</tr>
<tr>
<td></td>
<td>Mass Flow of Phase</td>
<td>(kg/h, t/h)</td>
<td>SMP(ID, pID)</td>
</tr>
<tr>
<td></td>
<td>Mass Flow of Component</td>
<td>(kg/h, t/h)</td>
<td>SMC(ID, cID)</td>
</tr>
<tr>
<td></td>
<td>Mass Flow of Element in Total</td>
<td>(kg/h, t/h)</td>
<td>SMET(ID, eID)</td>
</tr>
<tr>
<td></td>
<td>Mass Flow of Element in Phase</td>
<td>(kg/h, t/h)</td>
<td>SMEP(ID, eID, pID)</td>
</tr>
<tr>
<td>Mole Flow</td>
<td>Mole Flow of Total</td>
<td>(gmol/h, kgmol/h)</td>
<td>SNT(ID)</td>
</tr>
<tr>
<td></td>
<td>Mole Flow of Phase</td>
<td>(gmol/h, kgmol/h)</td>
<td>SNP(ID, pID)</td>
</tr>
<tr>
<td></td>
<td>Mole Flow of Component</td>
<td>(gmol/h, kgmol/h)</td>
<td>SNC(ID, cID)</td>
</tr>
<tr>
<td></td>
<td>Mole Flow of Element in Total</td>
<td>(gmol/h, kgmol/h)</td>
<td>SNET(ID, eID)</td>
</tr>
<tr>
<td></td>
<td>Mole Flow of Element in Phase</td>
<td>(gmol/h, kgmol/h)</td>
<td>SNEP(ID, eID, pID)</td>
</tr>
<tr>
<td>Concentration</td>
<td>Concentration of Phase in Total</td>
<td>As specified</td>
<td>SCPT(ID, pID, units)</td>
</tr>
<tr>
<td></td>
<td>Concentration of Phase in list of Phases</td>
<td>As specified</td>
<td>SCPP(ID, pIDs, units)</td>
</tr>
<tr>
<td></td>
<td>Concentration of Component in Total</td>
<td>As specified</td>
<td>SCCT(ID, cID, units)</td>
</tr>
<tr>
<td></td>
<td>Concentration of Component in list of Phases</td>
<td>As specified</td>
<td>SCCP(ID, cID, pIDs, units)</td>
</tr>
<tr>
<td></td>
<td>Concentration of Element in Total</td>
<td>As specified</td>
<td>SCET(ID, eID, units)</td>
</tr>
<tr>
<td></td>
<td>Concentration of Element in list of Phases</td>
<td>As specified</td>
<td>SCEP(ID, eID, pIDs, units)</td>
</tr>
<tr>
<td>Density</td>
<td>Density of Total</td>
<td>(kg/L)</td>
<td>SDT(ID)</td>
</tr>
<tr>
<td></td>
<td>Density of Phase</td>
<td>(kg/L)</td>
<td>SDP(ID, pID)</td>
</tr>
<tr>
<td>Volume Flow</td>
<td>Volume Flow of Total</td>
<td>(L/h, m³/h)</td>
<td>SVT(ID)</td>
</tr>
<tr>
<td></td>
<td>Volume Flow of Phase</td>
<td>(L/h, m³/h)</td>
<td>SVP(ID, pID)</td>
</tr>
<tr>
<td>Temperature</td>
<td>Temperature</td>
<td>ºC</td>
<td>ST(ID)</td>
</tr>
<tr>
<td>Pressure</td>
<td>Pressure Total</td>
<td>(kPa)</td>
<td>SPT(ID)</td>
</tr>
<tr>
<td></td>
<td>Partial Pressure of Gas Phase</td>
<td>(kPa)</td>
<td>SPP(ID, pID)</td>
</tr>
<tr>
<td></td>
<td>Partial Pressure of Gas Component</td>
<td>(kPa)</td>
<td>SPC(ID, cID)</td>
</tr>
<tr>
<td>pH</td>
<td>pH of a Phase</td>
<td></td>
<td>SHP(ID, pID)</td>
</tr>
<tr>
<td>Energy Flow</td>
<td>Internal Energy Flow</td>
<td>(kJ/h, MJ/h)</td>
<td>SU(ID)</td>
</tr>
<tr>
<td><strong>Equipment Properties:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Volume Flow</td>
<td>Stream maximum flowrate</td>
<td>(L/h, m³/h)</td>
<td>SMAXFLOW(ID)</td>
</tr>
<tr>
<td></td>
<td>Stream minimum flowrate</td>
<td>(L/h, m³/h)</td>
<td>SMINFLOW(ID)</td>
</tr>
<tr>
<td>Temperature</td>
<td>Specified temperature (when not energy balancing)</td>
<td>ºC</td>
<td>SSPECTEMP(ID)</td>
</tr>
<tr>
<td>Pressure</td>
<td>Specified/relief pressure</td>
<td>(kPa)</td>
<td>SSPECPRESS(ID)</td>
</tr>
<tr>
<td>Property Modes</td>
<td>Stream Property, command to change mode</td>
<td></td>
<td>SCHANGE(ID, propID, modeID)</td>
</tr>
<tr>
<td></td>
<td>Stream Property, current mode number</td>
<td>(#)</td>
<td>SMODE(ID, propID)</td>
</tr>
</tbody>
</table>
### Table 15-3: Other User Functions and Operations

<table>
<thead>
<tr>
<th>Categories</th>
<th>Description</th>
<th>Output Value Units</th>
<th>Syntax</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Instrumentation Operations:</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Timers</strong></td>
<td>Timer output value, countdown time remaining (h)</td>
<td></td>
<td>TO(ID)</td>
</tr>
<tr>
<td></td>
<td>Timer start, command to restart with specified countdown time in hours</td>
<td></td>
<td>TSTART(ID, time)</td>
</tr>
<tr>
<td><strong>Controllers</strong></td>
<td>Controller output value</td>
<td></td>
<td>CO(ID)</td>
</tr>
<tr>
<td></td>
<td>Controller, command to enable/disable</td>
<td></td>
<td>CSWITCH(ID)</td>
</tr>
<tr>
<td></td>
<td>Controller, command to zero integral error</td>
<td></td>
<td>CRESET(ID)</td>
</tr>
<tr>
<td><strong>Expressions</strong></td>
<td>Expression output value, current</td>
<td></td>
<td>EO(ID)</td>
</tr>
<tr>
<td></td>
<td>Expression, command to write specified value to</td>
<td></td>
<td>EWRITE(ID, expr)</td>
</tr>
<tr>
<td><strong>Expression Lists</strong></td>
<td>Expression List output value, current value of the next in list</td>
<td></td>
<td>LO(ID)</td>
</tr>
<tr>
<td></td>
<td>Expression List, command to increment active status to set expression at the specified index as active</td>
<td></td>
<td>LINCREMENT(ID)</td>
</tr>
<tr>
<td><strong>Simulation Parameters and Operations:</strong></td>
<td>Simulation, runtime (h)</td>
<td></td>
<td>TIME()</td>
</tr>
<tr>
<td></td>
<td>Simulation, command to end</td>
<td></td>
<td>EXITSIM()</td>
</tr>
<tr>
<td><strong>Constants:</strong></td>
<td>Pi</td>
<td></td>
<td>PI()</td>
</tr>
<tr>
<td></td>
<td>Gas constant, (J/K/mol)</td>
<td></td>
<td>R()</td>
</tr>
</tbody>
</table>

The way in which user functions reference equipment items, Phases and Components is summarised in the following key:
Table 15-4: User Function Syntax Key

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
<th>Legal Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>ID</td>
<td>Equipment ID</td>
<td>&gt;0 = Equipment ID number&lt;br&gt;0 = the equipment item calling the function (i.e. itself)&lt;br&gt;&lt;0 = the incoming datalink Port ID</td>
</tr>
<tr>
<td>piD</td>
<td>Phase ID</td>
<td>&gt;0 = Phase ID as per Component Database&lt;br&gt;0 = Parent Phase of nominated Component (where applicable)&lt;br&gt;-1 = all solid phases&lt;br&gt;-2 = all liquid phases&lt;br&gt;-3 = all gas phases</td>
</tr>
<tr>
<td>piDs</td>
<td>List of Phase IDs</td>
<td>e.g. 1,3,4</td>
</tr>
<tr>
<td>cID</td>
<td>Component ID</td>
<td>cID = Component ID as per Component Database</td>
</tr>
<tr>
<td>eID</td>
<td>Element ID</td>
<td>eID = element atomic number</td>
</tr>
<tr>
<td>units</td>
<td>Units of Measure</td>
<td>1 = w/w&lt;br&gt;2 = g/L&lt;br&gt;3 = v/v&lt;br&gt;4 = m/m&lt;br&gt;5 = gmol/L</td>
</tr>
<tr>
<td>propID</td>
<td>IPU Property ID</td>
<td>1 = Total Volume&lt;br&gt;2 = Overflow Volume&lt;br&gt;3 = Specified Pressure&lt;br&gt;4 = Specified Temperature&lt;br&gt;5 = Input Heat&lt;br&gt;6 = Input Work</td>
</tr>
<tr>
<td>propID</td>
<td>Controlled Stream Propert ID</td>
<td>1 = Flow Control&lt;br&gt;2 = Composition&lt;br&gt;3 = Maximum Flowrate&lt;br&gt;4 = Minimum Flowrate&lt;br&gt;5 = Temperature&lt;br&gt;6 = Pressure</td>
</tr>
<tr>
<td>modeID</td>
<td>Mode ID</td>
<td>1 to n</td>
</tr>
</tbody>
</table>

Mathematical operators and functions also available to the user are listed in the following table:
### Table 15-5: Mathematical Operators and Functions Available to Users

<table>
<thead>
<tr>
<th>Operator/Function</th>
<th>Description</th>
<th>Example Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>Add</td>
<td>1 + 1 = 2</td>
</tr>
<tr>
<td>-</td>
<td>Subtract</td>
<td>1 - 1 = 0</td>
</tr>
<tr>
<td>*</td>
<td>Multiply</td>
<td>2 * 3 = 6</td>
</tr>
<tr>
<td>/</td>
<td>Divide</td>
<td>6 / 3 = 2</td>
</tr>
<tr>
<td>&gt;</td>
<td>Greater than (numeric)</td>
<td>9 &gt; 2 = TRUE</td>
</tr>
<tr>
<td>&lt;</td>
<td>Less than (numeric)</td>
<td>7 &lt; 4 = FALSE</td>
</tr>
<tr>
<td>=</td>
<td>Equal test (numeric)</td>
<td>5 == 4 = FALSE</td>
</tr>
<tr>
<td>&gt;=</td>
<td>Greater or equal (numeric)</td>
<td>3 &gt;= 3 = TRUE</td>
</tr>
<tr>
<td>&lt;=</td>
<td>Less or equal (numeric)</td>
<td>11 &lt;= 9 = FALSE</td>
</tr>
<tr>
<td>&lt;&gt;</td>
<td>Not equal (numeric)</td>
<td>13 &lt;&gt; 20 = TRUE</td>
</tr>
<tr>
<td>IF</td>
<td>If condition</td>
<td>IIF(1+1==2, 4, 5) = 4</td>
</tr>
<tr>
<td>MIN</td>
<td>Minimum value</td>
<td>MIN(10, 3) = 3</td>
</tr>
<tr>
<td>MAX</td>
<td>Maximum value</td>
<td>MAX(1, 9, 2) = 9</td>
</tr>
<tr>
<td>SIN</td>
<td>Sine</td>
<td>SIN(PI()/2) = 1</td>
</tr>
<tr>
<td>COS</td>
<td>Cosine</td>
<td>COS(PI()) = -1</td>
</tr>
<tr>
<td>TAN</td>
<td>Tangent</td>
<td>TAN(1) = 1.5574...</td>
</tr>
<tr>
<td>ATAN</td>
<td>Arc tangent</td>
<td>ATAN(0) = 0</td>
</tr>
<tr>
<td>ABS</td>
<td>Absolute value</td>
<td>ABS(-8) = 8</td>
</tr>
<tr>
<td>EXP</td>
<td>e to the power of</td>
<td>EXP(3) = 20.08...</td>
</tr>
<tr>
<td>LN</td>
<td>Natural logarithm</td>
<td>LN(16) = 2.77...</td>
</tr>
<tr>
<td>LOG</td>
<td>Base 10 logarithm</td>
<td>LOG(100) = 2</td>
</tr>
<tr>
<td>CEIL</td>
<td>Round up</td>
<td>CEIL(6.2) = 7</td>
</tr>
<tr>
<td>FLOOR</td>
<td>Round down</td>
<td>FLOOR(3.3) = 3</td>
</tr>
<tr>
<td>SIGN</td>
<td>Sign (returns -1, 0, or 1)</td>
<td>SIGN(-9) = -1</td>
</tr>
<tr>
<td>SQRT</td>
<td>Square root</td>
<td>SQRT(64) = 8</td>
</tr>
</tbody>
</table>

### 16 Navigating the Model User Interface

The function of each command available on the menu bar in the Model tab is briefly described under the following headings. Most of these commands are also available as context menu items that appear when right-clicking on flowsheet sections and building blocks.

#### 16.1 File

**New**

Opens a blank model file.

**Open**

Opens a dialogue for selecting a model file (.ith) for opening.

**Save**

Saves the current model file, or requests a filename and save location if not already specified.
Save As…
Opens a dialogue requesting a filename and save location. Once nominated the model files are saved.

Print
Opens a print dialogue for printing the selected flowsheet section.

Print Preview
Provides a preview of what will be printed.

Page Setup
Opens a dialogue for changing print settings.

Close
Closes the current model. The user will be asked to save the file.

16.2 Components
Opens the Phases and Components screen.

16.3 Unit Operations

Add IPU
Adds an ITHACA process unit to the current flowsheet section.

Open IPU Menu
Opens the menu of the selected IPU.

16.4 Streams

Add Source
Adds a Source to the current flowsheet section.

Add Sink
Adds a Sink to the current flowsheet section.

Add Splitter
Adds a Splitter to the current flowsheet section.

Add Combiner
Adds a Combiner to the current flowsheet section.

Add Section Departure
Adds a Section Departure flag to the current flowsheet section.
Open Item Menu
Opens the menu of the selected Streams item.

16.5 Control & Instrumentation

Add PID Controller
Adds a PID Controller to the current flowsheet section.

Add Expression
Adds an Expression to the current flowsheet section.

Add Timer
Adds a Timer to the current flowsheet section.

Add Expression List
Adds an Expression List to the current flowsheet section.

Open Item Menu
Opens the menu of the selected Control & Instrumentation item.

16.6 Flowsheet

Add Section
Adds a flowsheet section to the model.

Delete Section
Deletes the current flowsheet section from the model after prompting the user to confirm this choice.

Duplicate Item
Duplicates the selected item.

Delete Item
Deletes the selected item after prompting the user to confirm this choice.

Activate Zoom
When zoom is activated, selecting around any part of a flowsheet section causes this selection to be increased in size to fit the main application window dimensions.

Reset Zoom
Resets the size of zoomed flowsheet sections to normal.

Show/Hide Datalinks
Shows or hides all Datalinks on a flowsheet section.
**Show/Hide Data Ports**
Shows or hides all Data Ports on a flowsheet section.

**Show/Hide Stream Ports**
Shows or hides all Stream Ports on a flowsheet section.

**Link From Selected Departure**
Active only if a Section Departure is selected. Opens a list of possible flowsheet sections to link to another section.

**Simulate/Ignore All Process Units**
Sets all IPUs on the current flowsheet section to either IGNORE or SIMULATE status, depending on the status of the first IPU interrogated.

### 16.7 Customisation

**Group**
Groups the selected items behind a single Default Group Icon.

**Ungroup**
Reverses a Group operation.

**Add Image**
Opens a dialogue for selecting an image file, for insertion in place of the current image displayed for the selected IPU or Group node.

**Remove Image**
Reverts an IPU or Group node to its default image.

**Lock/Unlock Ports**
Locks or unlocks Stream and Data Ports of the selected IPU or Group node. Unlocked Ports are indicated with a blue outline, and may be moved relative to their parent node. Locking fixes Port locations relative to the parent node.

**Add Model to Library**
If a Library is open and the model has a unique name in that library, then it is added.

**Libraries**
Opens the Equipment Model Libraries Manager.

**Open Menu**
Opens the selected Group item menu.
16.8 Visualisation

   Add Graph
   Adds a Single Variable Graph to the flowsheet.

16.9 f(x)
   Opens the user function quick reference window.

16.10 About
   Opens a small window in which displays information about ITHACA, the user licence and the user’s support status.

16.11 Units
   Selection menu for the magnitude of the units in use.

16.12 Gas Model
   Selection menu for the gas model to apply. Currently only the ideal gas model is available.

16.13 Colour Scheme
   Select from Dark or Light flowsheet section background colour.

16.14 Show Grid
   Show or hide the grid.

17 Simulation
   Once a model is ready to be simulated, follow these steps:
   1. Save the model
   2. Switch to Simulate view
   3. Select the desired options from the following tick-boxes:

   ![Simulation Options]
   Generate Result Files can also be selected during simulation but the other options cannot.

   4. Specify the time period to be simulated in the following fields:

   ![Simulation Time]
   These values can also be edited during simulation.

   5. Left-click the button. To pause the simulation left-click and to terminate the simulation click .
17.1 Configuring Solver Parameters

ITHACA simulations are driven by a powerful variable step-size, globally convergent Newton solver that works together with an event management engine. Various parameters that affect the performance of these program elements are editable by the user.

Left-click Configure Solver in the Simulate view menu bar. The default values are suitable for most scenarios and can be reinstated by clicking the Defaults button.

**Minimum Time Step Size**

The smallest time step-size that will be taken during solving of continuous regions of the simulation. If the solution cannot be found with a step size of at least this minimum value then a message is displayed and the simulation is terminated. This is usually a sign of a model setup error, but can also mean a mathematically stiff region was encountered that simply needs a small minimum step size for the solver to navigate.

**Maximum Time Step Size**

The maximum time step size that the solver will take.

**Maximum Step Expansion Factor**

The maximum rate at which time step-size will be increased.

**First Step Size Fraction of Maximum**

The size of the first step attempted after a simulation discontinuity.

**Balance Error Tolerance**

The relative maximum mass and energy balance error allowed in any one time step across any single IPU, calculated as follows in the case of mass:

\[
error = \frac{m_{t_{n-1}} + \int_{t_{n-1}}^{t_n} (\dot{m}_{in} - \dot{m}_{out}) \, dt - m_{t_n}}{m_{t_{n-1}}}
\]

Where:

- \( m \) = mass
- \( \dot{m} \) = mass flow
- \( t \) = time
- \( n \) = \( n^{th} \) step

The smaller this balance error tolerance value is the harder the solver will work to achieve a solution within tolerance at each time-step. In general the largest tolerance that does not produce erroneous results is the best choice, however this is a subjective concept since any numerical solution will contain some degree of error. One method of arriving at a reasonable compromise is to reduce balance error tolerance until the resulting simulation solution does not change appreciably; however, for a long-duration simulation this may not be practical.
**Event Cross Error Tolerance**

Determines how close the event finder needs to get to an actual event time before the simulation can continue. The smaller this value is the harder the event finder will work to find the time at which an event occurred.

**Solver Error Tolerance**

The Newton solver requires an absolute and a relative error tolerance value for assessing the success of each iteration. The smaller these values are the harder the solver will work at each time step before being satisfied with a solution.

**Solver Maximum Chord Steps**

The Newton solver uses a Jacobian matrix to determine the direction and magnitude of the change to make to each simulation variable at each step of its estimation cycle. Calculation of the Jacobian is computationally expensive. When the solver takes a chord step it applies the Jacobian calculated in an earlier iteration to the current iteration, saving the time required to recalculate the Jacobian if the solution is found. This parameter controls the maximum number of chord steps allowed before the Jacobian is recalculated.

**Solver Maximum Newton Iterations**

This parameter controls how many attempts the solver will make to find a solution before it gives up and reduces the time step size.

**Multithreading**

Some computationally intensive operations are by default divided over the maximum number of available processors. Here the user can switch this feature off or reduce the number of processors used.

### 17.2 Simulation Live Views

**Global Error**

Global error is calculated in the same way as the IPU balance error calculation illustrated earlier with the exception that the balance is calculated across the flowsheet as a whole. The cumulative value of this error for any given simulation can be viewed by left-clicking the **Global Error** button in the Simulate view menu bar during simulation.

**Solver Parameters**

A limited view of solver parameters is available by clicking **View Solver** in the menu bar. The view shows the live state of the solver error for each new estimation of the solution; a brief text description of the current stage of solution; and a visualisation of the non-zero entries in the Jacobian matrix.

**Process Data Visualisation**

Live simulation data can be visualised in two ways: by setting up Single Variable Graphs during the model building phase or by double-clicking any IPU or stream during simulation.
Single Variable Graphs present the value of a single variable or calculation either as a trendline or as a column chart. These charts show a limited number of data points in order to avoid exhausting computer memory during long simulations.

When an IPU or stream is double-clicked a multi-tab window opens to display comprehensive information about the contained phases and components. Data is not sent to these charts until they are opened.

### 17.3 Data Output

If **Generate Result Files** is selected in the SIMULATE menu bar then simulation data is output to Excel (.xlsx) files. During simulation a data file is created once the accumulated data in memory reaches a predetermined quantity. Once written to the Excel file the data in memory is then overwritten with subsequent simulation data. A final data file is generated at the end of the simulation.

Each data file is named with the UTC date and time to guarantee unique filenames, and saved to the model's results folder.

Multiple data files can be programmatically compiled into a single Excel file using a free tool developed by Element Process Technology. Please [contact us](mailto:contact@elementprocesstechnology.com) if you are interested in this tool.

If a data file is required for viewing during simulation then clicking **Get Interim Result** will generate a data file containing the data set currently held in memory.

### 18 Monte Carlo Simulation

When a model makes use of stochastic inputs then each simulation is likely to produce a different result, and the probability of that result occurring is related to the probability assigned to the stochastic inputs together with the configuration of the flowsheet. One method of quantifying the probability of certain results occurring is by running multiple (hundreds or even thousands) of simulations. This method is called Monte Carlo simulation.

A typical application is determining the likelihood of a water containment pond overflowing given stochastic input rainfall and evaporation rates. In this example rainfall may be set daily with an appropriately selected density function reflecting the likelihood of a range of rainfall rates possible for that day.

Monte Carlo simulation is only realistic (with regards to time take to complete) for relatively simple flowsheets, ie those with a minimum of IPUs and components.

Data output from Monte Carlo simulations are limited to a small number of user-determined parameters. To set up Monte Carlo simulation first set up an Expression (deterministic mode) for each parameter of interest. Check the **Activate** box in the Monte Carlo panel on the SIMULATE tab, then click **Setup**. A list of all Expression elements on the flowsheet will be presented. Select those whose output you wish to record during simulation and specify the number of simulations required.

Results can be presented as interpolated, raw or both. In order to compare results across simulation runs, for example to plot a histogram and determine probability percentiles of outcomes, interpolation is required. Raw data can be of interest in trouble-shooting a flowsheet but is generally not required otherwise. The user selects the interval of interpolation,
for example hourly, 2-hourly, daily, etc, as appropriate. The smaller the interpolation interval the better resolution will be had on results, but the more data there will be to store and manipulate.

Once set up, Monte Carlo simulation is initiated simply by clicking the play button, as per a normal simulation. Output of the datafile occurs after all simulations are complete, unless the volume of data is so great that an intermediate result file is also produced.