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Technical Note – Atlas Software Quick Start Guide

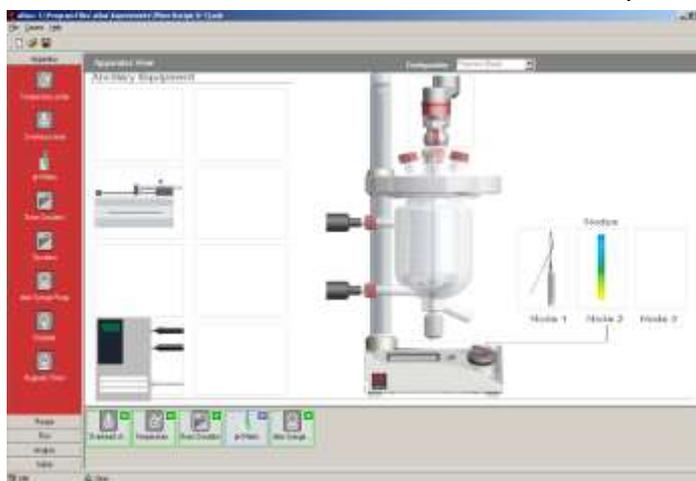
1.1 Introduction

The Atlas software is based around a **3 screen system**. Further screens allow for offline analysis and system management.

View	Description
Apparatus	The Apparatus view allows user to specify what is connected to Atlas to be used in the reaction.
Recipe	The Recipe view defines what reaction steps Atlas will complete to perform the process.
Run	The Run view displays the reaction progress, the apparatus status and real-time data.
Analysis	The Analysis view allows datalogs and corresponding recipe's to be viewed graphically in the software.
Admin	The Admin view allows an administrator to configure the Atlas software.

1.2 Starting the software – Apparatus view

Atlas automatically detects the number of ports and nodes present in the system and will only allow devices to be added to available connections. Devices can be added to port connections by dragging them from the left hand list to the main window. Devices can be added to node connections by dragging them onto the node ports labelled on the right hand side of the screen.





Apparatus can be added by either, selecting and dragging the icon onto the apparatus view, or by double clicking on the icon in the navigation bar. Either of these actions will launch a device properties window. Here it is possible to set a maximum and minimum limit for the device and to enable the use of limits. The safe value is the value to set the device to in case of emergency (or at the end of an experiment). The sensors associated with the apparatus can be viewed from the sensors tab. Alarms can be configured here to give warnings when certain high/low values are reached. Automatic shutdown values can also be set.

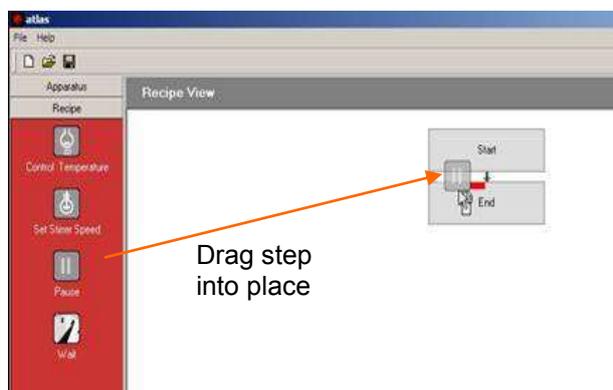
The apparatus list is shown at the bottom of both the apparatus and recipe views. It shows the apparatus currently set-up within Atlas and the status.



As apparatus is added it is shown with a blue question mark (as above) showing that although the apparatus is configured, Atlas doesn't have an associated recipe step for it.

1.3 Recipe view

The recipe view allows the user to design, edit and configure a reaction in individual steps by means of a flow-chart format. Recipe steps can be dragged from the list on the left onto the diagram in the centre of the recipe view, to form a process.

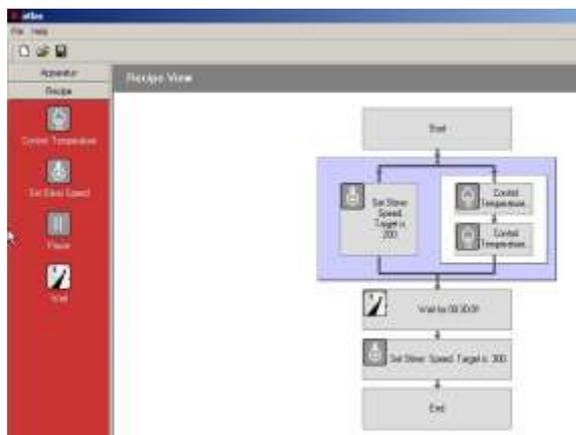


The example (left) shows a step being dragged to the end of the experiment. Steps can be added before, after or in parallel with other steps (as shown below). After dragging a recipe step onto the recipe view a step properties window will be launched to define the exact method, targets, and end conditions associated with it.

Sequential steps will happen in order, one after the other. Concurrent steps happen at the same time as each other. Note that in this example the wait step will not start until all the steps within the blue background have been completed.

Steps can be moved by dragging them from their current location to a new location.

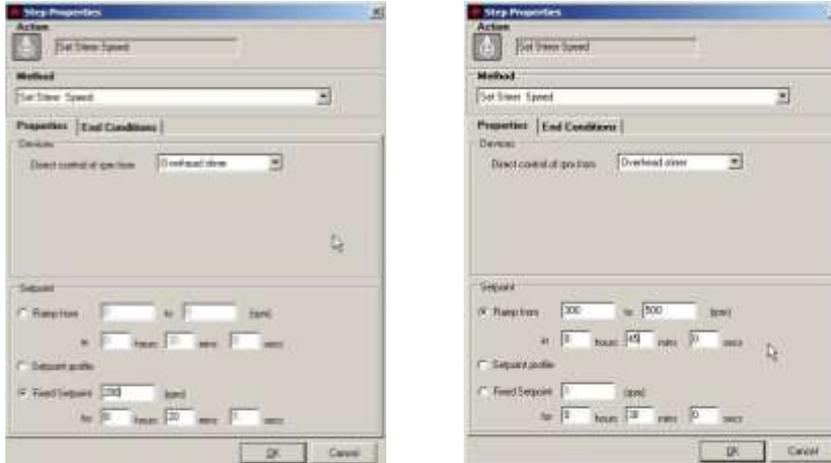
Right clicking on any step produces a menu where steps can be deleted, edited, duplicated and their properties viewed. Duplicating steps creates a direct copy (including step



properties).

1.3.1 Recipe step properties

Recipe step properties are displayed when a step is first added to the recipe or by double clicking on an existing step



There are then a number of options listed. The “fixed set point” option allows users to specify both a target point and duration.

The ramp from/to option allows a constantly moving set point to be defined over a specified period.

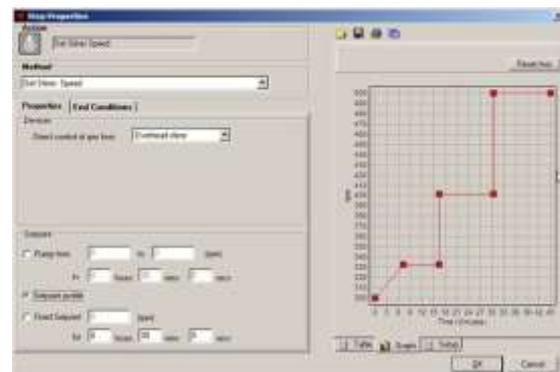


Set point profiles can be defined in two ways. They can either be added in the form of a table or graph. Selecting “set point profile” enables the profile editor.

- The table view allows specific time points to be defined.
- The time and value can be entered.

The graph view allows points to be created and moved around.

- Double clicking on the graph will create a new node which can then be dragged to create a new set point/ramp.
- Dragging outside the bounds of the current axis limits will scroll the display.



1.3.1.1 End conditions



- As part of the step properties users can specify end conditions for the step. These can be based on the system achieving the set point, another sensor reading or after a fixed time.
- End on final point allows users to specify that the endpoint should be above, below or within a certain range of the set point.
- End on other sensor allows the system to “tare” the sensor at the beginning of the step which can be used with balances when the addition of a certain mass is required.
- “End after time” will override the set point.

1.3.1.2 Step limits

- Step limits allow definition of limits for the specific recipe action step, regardless of the overall device limits. This function provides a safety control for each recipe action step e.g. the device limits may be set to min -10°C and max 100°C, but the first stage is at 20°C. The Limit properties min output may be set to 15°C and the Limit properties max output to 25°C. This will then control the circulator within these limits for this step of the reaction.



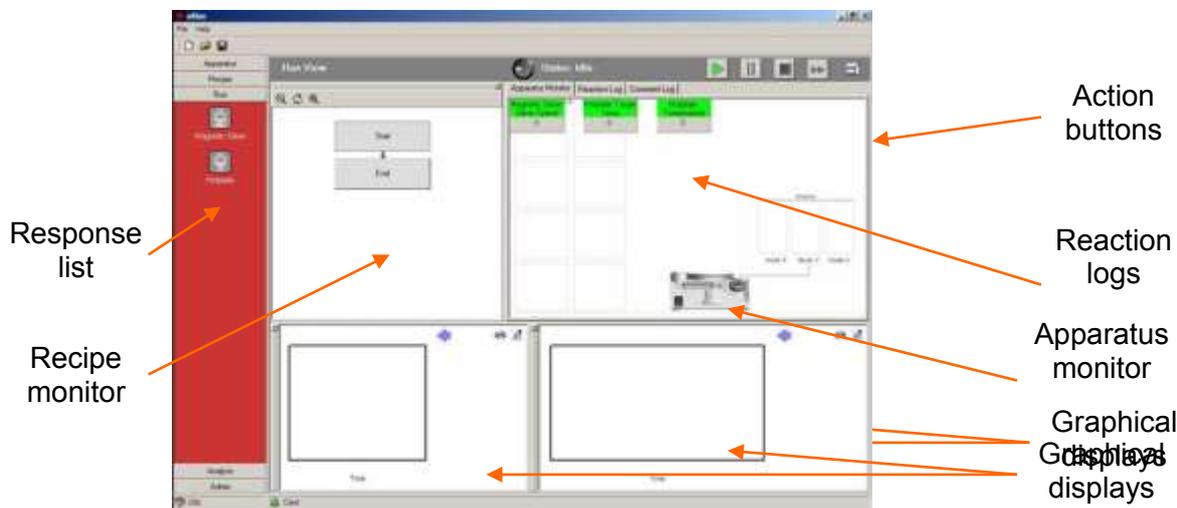
1.3.1.3 PID



- PID parameters for specific steps can be defined. These are advanced settings and should not be modified except by experienced users. They can be used for example to adjust the PID response to a particular fill level (to stabilise control when small volumes are used or to increase power when large volumes are needed).
- Details on PID parameters can be found in section **Error! Reference source not found.** of the full Atlas manual

1.4 Run view

The run view enables experiments to be started, monitored, paused or stopped.



- The recipe monitor shows the progress of an experiment through the defined steps.
- The apparatus monitor displays all the instrument responses being measured in addition to all of the set points which are defined.
- The graphical displays allow responses and set points to be plotted vs. time..
- The action buttons allow experiments to be started, stopped, paused or individual steps skipped.
- The response list shows which responses are available to be added to the graphs.
- The reactions logs show historically what has occurred in text form. The reaction log contains all the steps which have occurred whilst the experiment log allows users to note their own observations or manual changes.

The action buttons at the top of the run view are used to start, stop and pause experiments. Below is a summary of their function.

Icon	Function
	Click 'Run' to Validate and Run the reaction.
	Click 'Pause' to pause and resume the reaction. All devices will switch to their predefined paused states. The state could be set to maintain current value or set to a default value.
	Click 'Stop' to halt the reaction and to set all devices to safe.
	Click 'Skip all active steps' to stop all active Recipe steps and to move on to the next step.
	Click to reset all the docked windows to their default locations.

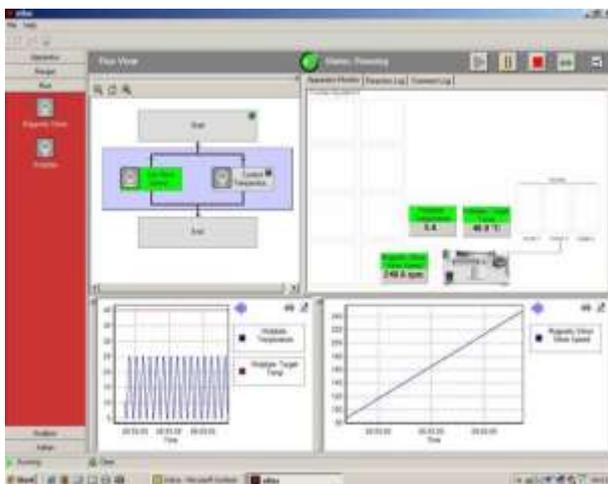
Pressing the start button at the top of the run view will start the experiment. Atlas will first verify the experimental procedure to ensure that it is both logically correct and that all the required equipment is correctly defined.

Experiments can be paused at any point by pressing the pause button. This will hold any ramps currently being applied and maintain any set points to enable users to make changes

to the process. Whilst an experiment is paused the recipe view can be accessed to allow users to change the defined process.

Stopping an experiment before it has reached completion can be performed by pressing the stop button.

1.4.1 Real-time graphical displays



- Graphs can be added to the run view by dragging items from the response list on the left onto an existing graph or by double clicking on an item to add a new graph.
- Additional responses can be added to an existing graph by dragging the response onto that chart.
- Where two or more responses correspond to the same hardware a dialogue box will allow users to select the required response

1.4.2 Exporting data

All Atlas data is saved in comma separated value format (.csv). This format is readily imported into most major spread sheeting packages (e.g. Microsoft Excel or OpenOffice Calc). A header row is included to enable analysis and graphing of the correct responses. Data files are saved into a “logs” directory in the c:\program files\Atlas unless previously defined in the admin view. The default file name is a time-stamp again unless the administrator has requested that files be named at the time of creation.

1.4.3 Modifying a reaction in progress

Users can use the pause function to modify experimental parameters or process whilst an experiment is running. This can be done in one of two ways; either by pressing the pause button and changing to the recipe view or by double clicking on the step you wish to change. (Note only the recipe, run and analysis views are available whilst an experiment is paused).

If the pause button has been used to modify parameters new steps can be added to the recipe in addition to the ability to change the set point from the current step.

When the reaction is un-paused Atlas will revalidate the process to ensure that there are no illegal steps.

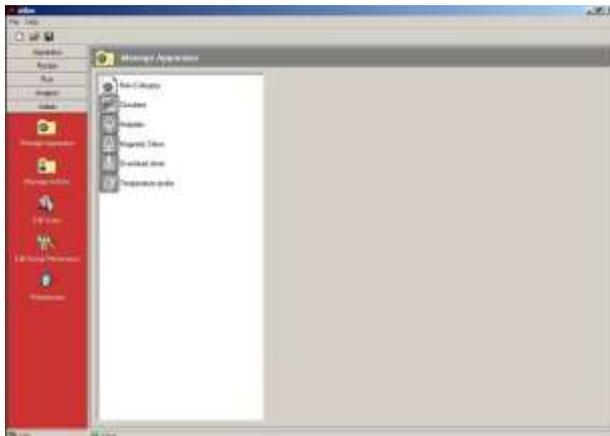
1.5 Analysis view



Analysis view enables experiments to be viewed and analysed post-run. Data logs can be selected and loaded and if available an associated experiment file can be loaded to provide further information.

The analysis view works in a similar way to the run view in that, instrument responses can be selected from the bar on the left and dragged onto charts. Several different responses can again be viewed on a single graph and these can be toggled on and off by clicking on the graph legend.

1.6 Admin view



The admin view enables users to add new apparatus, define new recipe steps, define permissions and set software preferences. It is only possible to access this view when logged in as an administrator

- Specific preferences include those pertaining to data logging, instrument configuration, graphical displays, and alert settings.