Benefits and Applications

The Atlas Reaction Calorimeter has the following benefits:

- **Fully automated**
- **Excellent control**
- **Accurate**
- **Walk away operation**
- **Wide temperature and pressure range**
- **Easy analysis**
- **Quick to set up**
- **Flexible**
- **Safe**
- **Compact**

Above: Quick response RTD probe measures the temperature of the jacket (Tj)

Left: Heat Flow Calorimetry configuration with gravimetric dosing

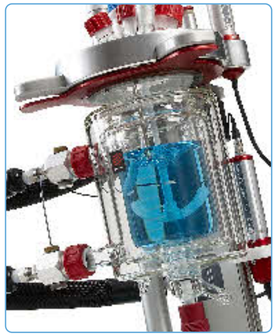
Atlas Reaction Calorimeter has the following applications:

- **Process development**
- **Safety**
- **Kinetic studies**
- **Scale-up**
- **Parallel chemistry**
- **Process optimization**
- **End point detection**

Atlas - The Best Value Process Reactor in the World!

The Atlas Calorimeter is one product within the Atlas range of automated reactor systems. Atlas is a revolutionary range of modular products, which can form a wide range of chemical reactors. Atlas offers manual or automated control of one or many reactions at a time with volumes from 5 litres to 1ml in jacketed reactors, flasks or vials.

Atlas applications include synthesis, calorimetry, process optimization, crystallization control, automated addition or pH control, high pressure reactions, parallel chemistry and many more.



Atlas Benefits

- **Easy to use:** Twist & click knob, large display and intuitive
- **Automated:** Walk away synthesis
- **Full data capture:** Data automatically recorded by Atlas Base (downloadable by USB memory stick) or PC software
- **Quick:** Everything clicks together quickly and easily without tools.
- **Small footprint:** 23cm (9") square easily fits in fume cupboards
- **Robust:** Specifically designed for use in chemical laboratories
- **Safe:** Auto shutdown, alarms and safe touch surfaces

Watch the Atlas videos at www.syrris.com/videos

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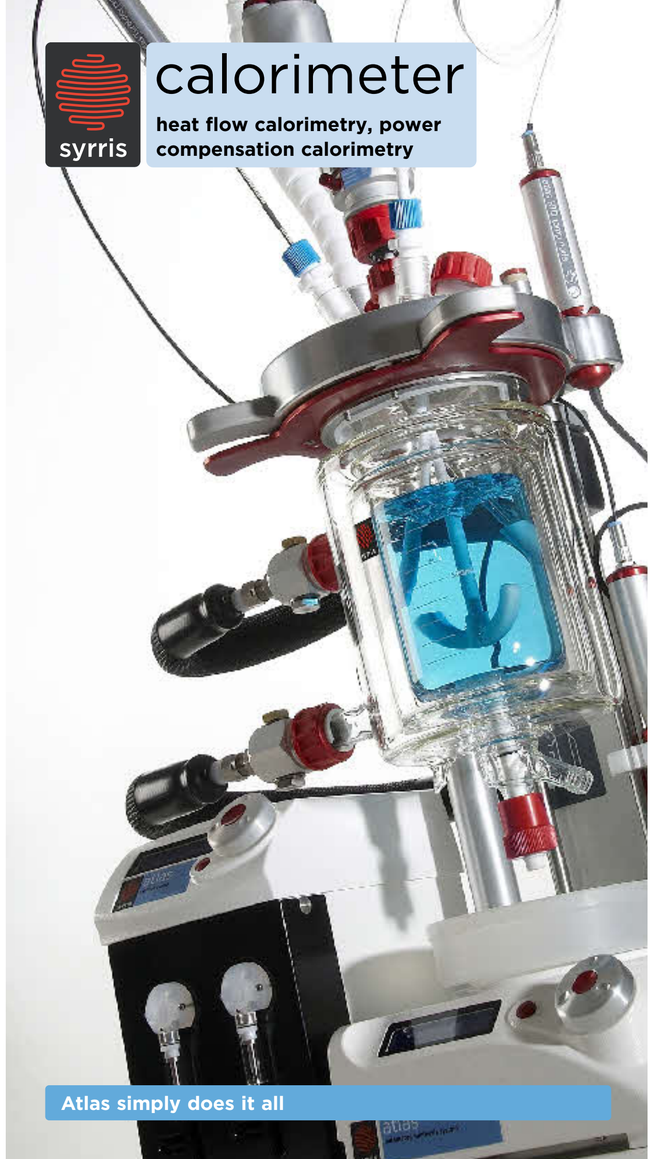
calorimeter

heat flow calorimetry, power compensation calorimetry



Atlas simply does it all

What is the Atlas Reaction Calorimeter?

The Atlas Reaction Calorimeter accurately measures the power and enthalpy of chemical reactions. This provides information such as reaction kinetics and safety data that is invaluable in process optimization, scale-up and hazard analysis.

Atlas Calorimeter Specification

Interchangeable jacketed reaction vessels	100ml, 250ml, 500ml, 1 litre and 2 litre vacuum jacketed reactors available with a range of profiles including round, torispherical, conical or custom.
Temperature range	-40°C to 150°C recommended for calorimetry (up to 200°C possible).
Accuracy	Typically 1 to 5% (dependent on settling time and external conditions) .
Calorimetric techniques used	Heat flow calorimetry (HFC) or power compensation calorimetry (PCC).
Footprint	From 40cm (16") wide.
Chemical resistance	Glass, PTFE and other fluoropolymers.
Maximum reaction power	100W/litre maximum (50W for power compensation calorimetry).
Safety features	Warnings, alarms and automatic shutdown can be set for the whole experiment and each process step.
Stirring options	Anchor, pitched blade propeller, retreat curve impeller or custom made in glass or PTFE. 0-800RPM (up to 11Ncm) or 0-1000RPM (up to 90Ncm) with torque feedback.
Circulator options	Julabo, Huber, Lauda, Haake
Equipment supplied	Standard Atlas Potassium System, plus: Atlas PC Software Atlas Calorimetry Software Upgrade and Atlas Reporting Software Atlas Port for recirculator control Vacuum jacketed vessel (see above) Fast response reaction temperature probe T_j (jacket in) measurement probe with node and insulated cover PC controlled heater power supply with Atlas Port Reactor heater
Dosing options	Manual dosing, Atlas Syringe Pump for automatic volumetric dosing or peristaltic pump and balance for gravimetric dosing.
Other sensor options	pH, in-situ FTIR sensor, turbidity, pressure, etc.

Heat Flow and Power Compensation Calorimetry

The Atlas Calorimeter has been designed so heat flow calorimetry (HFC) and power compensation calorimetry (PCC) are performed with the same equipment, allowing a choice of methods for the reaction.

Heat Flow Calorimetry (HFC) or Power Compensation Calorimetry (PCC)?

HFC is generally used for reactions where the heater may have an effect on the chemistry, since the dip in heater is not used during the reaction. HFC is also preferred when large exotherms are expected.

PCC is used where quicker results are required, since no pre and post calibration is required.

Data can be shown in real time with both methods using Atlas.

Power Compensation Calorimetry (PCC)

PCC provides a very direct method for measuring process power and enthalpy.

The reactor runs isothermally with the jacket set at a constant temperature below the desired reaction temperature. The temperature offset is maintained by the addition of power.

The energy input is adjusted continuously by the Atlas Software to maintain the reactor contents at the desired temperature.

PCC determines the heat of reaction by monitoring the power supplied to a compensation heater placed in the reactor (above).

Heat Flow Calorimetry (HFC)

HFC determines the heat flow into or out of the system by measurement of the temperature difference between the vessel jacket and the reactor.

The reactor temperature is controlled isothermally at all times by modulating the jacket temperature and the difference between the reactor temperature and the jacket temperature is monitored.

Data is gathered by measuring the difference between reactor temperature (Tr) and jacket temperature (Tj). The result (Tr-Tj) is a measure of the heat flow between the reactor and the jacket, is directly proportional to the actual power and is automatically calibrated before and/or after the experiment.

Why use the Atlas Calorimeter?

Accurate

A major (top three) pharmaceutical company independently tested the Atlas Calorimeter System using heat flow calorimetry (HFC) and power compensation calorimetry (PCC). They performed a range of endothermic and exothermic processes. The results of the experiments are shown below.

Real time data with no extra effort

Reaction calorimetry is a non-intrusive, non-destructive, real time technique that yields valuable process data. Historically, reaction calorimeters were too expensive, too difficult to operate or too slow to set up. The Atlas Calorimeter generates calorimetry data with the same effort required to run a regular experiment.

Independent Data

Experiment name	Literature value ΔH (kJ/mole)	Atlas value ΔH (kJ/mole)	Atlas Calorimeter technique used	Accuracy
Sensible heat of addition [1]	+6.06	+5.91	PCC	97.5%
Hydrolysis of Ac_2O in H_2O [2]	-56.6	-54.1	PCC	95.6%
Dissolution of NaOH in H2O [3]	-44.51	-44.51	HFC	100%
Hydrolysis of Ac_2O in H_2O [2]	-56.6	-53.51	HFC	94.5%

1 50ml of H_2O added to 150ml of H_2O at 50°C over 10 minutes
2 16g of Acetic anhydride added to 200ml of H_2O 50°C over 10 minutes
3 15g of Sodium hydroxide pellets added in one portion to 150ml of H_2O at 25°C

The Atlas Calorimeter System

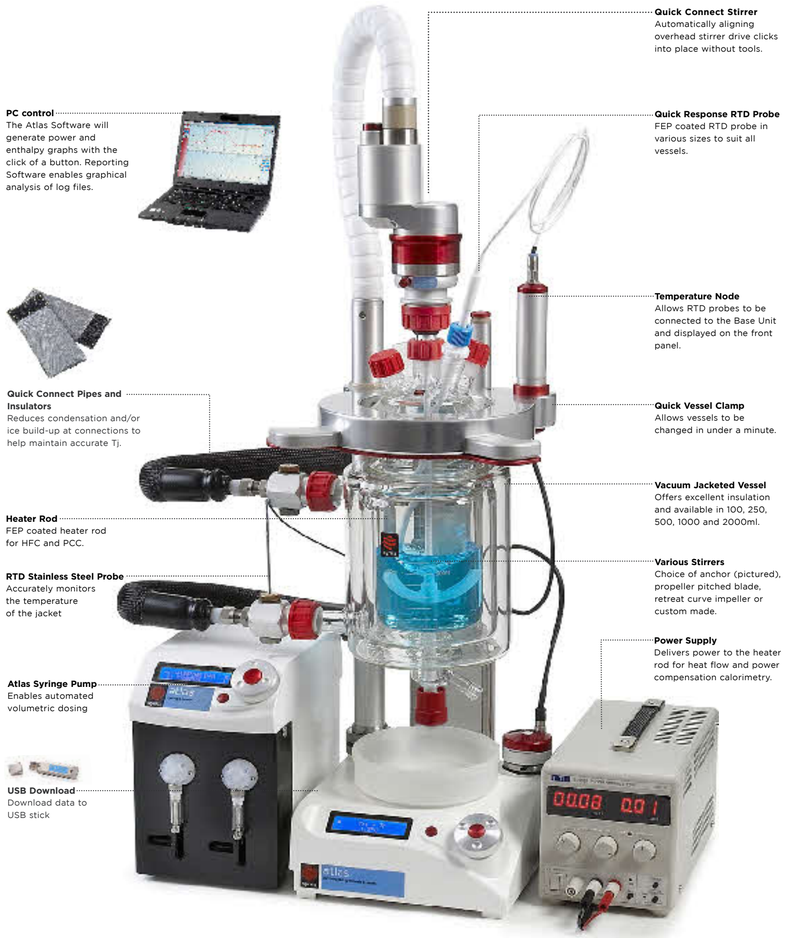
The Atlas Calorimeter system allows reactors of 100ml, 250ml, 500ml, 1L or 2L to be interchanged in under a minute. All sensors, stirrers, pumps, etc. are automatically detected and easily controlled, allowing quick upgrade of functionality. Options include automated liquid addition, pressure reactions, and sensors such as pH, turbidity or in situ FTIR.

Atlas Calorimeter Options

FTIR Analysis
The addition of a Bruker Matrix Spectrophotometer allows the Atlas Calorimeter to be upgraded to include FTIR analysis.

High Pressure
The addition of a pressure vessel with valves, cooling coils, burst disc and various other components allows the Atlas Calorimeter to be upgraded for high pressure applications.

High Torque Stirring
The addition of a Heidolph Stirrer and Heidolph stirrer adaptor kit allows the Atlas Calorimeter to be upgraded for applications that require high torque stirring.



PC control
The Atlas Software will generate power and enthalpy graphs with the click of a button. Reporting Software enables graphical analysis of log files.

Quick Connect Pipes and Insulators
Reduces condensation and/or ice build-up at connections to help maintain accurate Tj.

Heater Rod
FEP coated heater rod for HFC and PCC.

RTD Stainless Steel Probe
Accurately monitors the temperature of the jacket

Atlas Syringe Pump
Enables automated volumetric dosing

USB Download
Download data to USB stick

Quick Connect Stirrer
Automatically aligning overhead stirrer drive clicks into place without tools.

Quick Response RTD Probe
FEP coated RTD probe in various sizes to suit all vessels.

Temperature Node
Allows RTD probes to be connected to the Base Unit and displayed on the front panel.

Quick Vessel Clamp
Allows vessels to be changed in under a minute.

Vacuum Jacketed Vessel
Offers excellent insulation and available in 100, 250, 500, 1000 and 2000ml.

Various Stirrers
Choice of anchor (pictured), propeller pitched blade, retreat curve impeller or custom made.

Power Supply
Delivers power to the heater rod for heat flow and power compensation calorimetry.

Atlas Calorimeter Options

Turbidity Sensing
The addition of an Atlas Turbidity Node and Probe allows the Atlas Calorimeter to be upgraded to include Turbidity sensing.

pH Monitoring
The addition of an Atlas pH and Temperature Node and Probe allows the Atlas Calorimeter to be upgraded to include pH monitoring.

Gravimetric Dosing
The addition of a balance and a peristaltic pump allows the Atlas Calorimeter to be upgraded to include gravimetric dosing.

Reaction Calorimetry has Never Been so Simple

The Atlas Calorimeter is designed for ease of use. Setting up a system, running an experiment with software and then analysing the data using the innovative Atlas Reporting Software are all made easy with the Atlas Calorimeter.

Set-up System

The standard hardware required for a power compensation calorimetry (PCC) system and a heat flow calorimetry (HFC) system is the same.

All parts can be put together quickly and easily without the need for tools. Mechanical connections click firmly into place and electronic connections such as sensors and pumps are detected automatically.

The Atlas system connects to the PC by a USB cable.

Define Experiment

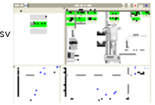
The Atlas Software has been designed to make defining, running and processing data from experiments, quick and easy.

Defining an experiment could not be more simple. The drag and drop interface allows you to select the modules you want to use, e.g. circulator, power supply, temperature probe, etc. and add them to your experiment apparatus.

From here you can easily define the desired calorimetry method (PCC or HFC), reaction temperature, quantity and rate of reagents to be dosed and experiment time, etc.

Run Experiment

When running the experiment, everything is controlled automatically including stabilization at desired reaction temperature, reagent addition and in the case of HFC, pre and/or post run calibration (no user intervention is required during the entire process).



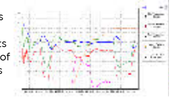
All data is continually logged to a common csv file and displayed by the software in graph format in real time.

Real time analysis is made easy by the Atlas Software featuring "single click" plotting of power and enthalpy. Comments can be added and the experiment paused and restarted during the process.

Process Data

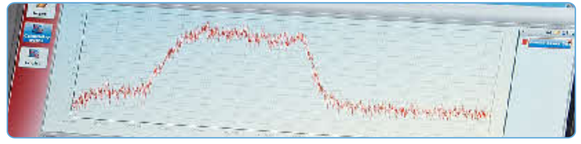
Processing data is simple with the Atlas Reporting Software which enables log files generated by Atlas Calorimetry Software to be interpreted quickly.

The software's wizard style interface allows fast and effective analysis of the thermal properties of the reaction with the click of a button.



The Software imports raw data and automatically corrects for the sensible heat of addition and changes in UA.

Graphs of reaction power/enthalpy, overall process enthalpy, and sensible heat of addition are instantly displayed with other process data such as additions.



Above: Atlas Reporting Software graphically displaying calorimetric data

Far left: Reaction control with PC software

Left: Analyse power and enthalpy data with Reporting Software