Parr Instrument Company

Stirred Reactors and Pressure Vessels

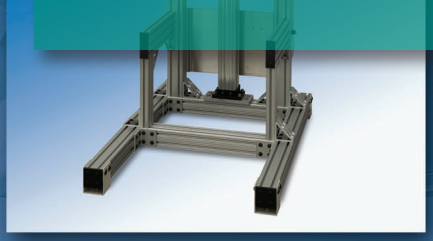
Bulletin 4500 | Volume 14

Designing and Building Quality Pressure Apparatus for Over 100 Years

Start

Chapter Three

This pdf is just one chapter from our Catalog 4500. Please refer to all eight chapters to make the proper equipment choice for your needs.



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Chapter 3

Multi Reactor Systems

Inside this chapter you will find:

5000 MULTIPLE REACTOR SYSTEM (MRS)

COMBINATORY CHEMISTRY AND HIGH-THROUGHPUT SCREENING SYSTEMS

5000 Multiple Reactor System (MRS)

Series Number:
5000

Type:
Multiple Vessel

Stand:
Bench Top

Vessel Mounting:
Moveable

Vessel Sizes, mL:
45 and 75

Standard Pressure MAWP, psi (bar):
3000 (200)

Standard Maximum Operating Temp., °C:
225 w/ FKM O-ring
300 w/ FFKM O-ring
300 w/ PTFE Flat Gasket

Model 5000 Multiple Reactor System, six 75 mL Vessels with Flat Gaskets and Head-Mounted Valves, shown with included 4871 Process Controller.

The Parr Series 5000 Multiple Reactor System has been designed to provide an integrated system for running multiple reactions simultaneously and applying the principles of high throughput experimentation to reactions conducted at elevated temperatures and pressures.

The principal features of the 5000 System include:

- Six reactors with internal stirring.
- Operating pressures to 3000 psi.
- Operating temperatures to 300 °C.
- Individual temperature control.
- Continuous individual pressure monitoring.
- Computer control and data logging.
- Manifold system for rapid turn around and to allow two different input gases.
- Volumes and reactor geometry designed for three phase reactions.
- Flexible Control Software.

Stirred Batch Reaction Vessel

This multiple reaction system has been designed around a vessel with 75 mL total volume. This will accommodate between 15 mL and 40 mL of liquid reactants which is close to the minimum volume appropriate for heterogeneous catalytic reactions.

The vessel valves and accessories are designed for maximum operating pressures up to 3000 psi at operating temperatures up to 300 °C. A system with 45 mL vessels is also available.

Stirring System

All six vessels are stirred with a single magnetic stirrer system specifically designed and built for this application. The magnetic drives and fields are focused on the stirrer bars within each vessel. High strength compact magnets are used to provide coupling forces which will operate through the heaters and vessels. The stirring speed of the stirrer bar is variable from 0-1200 rpm. All vessels will have the same stirring speed during a single run of the apparatus. This arrangement ensures that the difference in reaction rates between vessels run in parallel are due to set conditions other than variations in stirrer speed.

Heaters

The external heaters surround the vessel walls for rapid and uniform heating and temperature control. Each vessel is individually temperature controlled. The 250-watt heater used on each vessel produces heating rates up to 15 °C per minute. An optional reactor cooling support rack is available for air-cooling.

Series 5000 Pressure Reactor System Specifications				
Shaded bar indicates specifications that change within series.				
Model Number	**5000**			
Sizes, mL	45		75	
No. of Reaction Vessels	6			
Maximum Pressure	3000 psi (200 bar)			
Maximum Temperature				
with FKM O-ring	225 °C			
with FFKM O-ring	300 °C			
with PTFE Flat Gasket	300 °C			
Closure				
with O-ring	Screw Cap			
with Flat Gasket	Screw Cap (6 Compression Bolts)			
Material of Construction	T316SS			
Process Controller	Model 4871			
Analog Inputs	6 Temperature			
	6 Pressure			
	1 Motor Speed			
Analog Outputs	1 Stirrer Speed (Optional)			
Digital Outputs	6 PID Temperature Control			
Temperature Measurement	6 Thermowells			
Heater Style	6 Band Heaters, Aluminum Block			
Heater Power Watts	250W Per Station, 1500W Total			
External Thermocouple	Optional			
Stirrer Motor Type	Manual or Computer Controlled			
Stirrer Style	PTFE- or Glass- Coated Magnetic Stirrer Bar			
Electrical Supply				
Volts, AC	115 or 230			
Maximum Load, amps	15 / 7.5			
Vessel Dimensions				
Inside Diameter, inches	1.18		1.50	
Inside Depth, inches	2.69 Flat Gasket, 2.50 O-ring			
Weight of Vessel, pounds	3 (w/ Panel-mounted valves)		6 (w/ Head-mounted Valves)	
Dimensions	Width, in.	Depth, in.	Height, in.	Weight, lb.
Heater	25.75	9.25	2.875	31
Stirrer	28	9.5	7.625	12
4871 Controller	13	11	15	14
Manifold, Remote	26.5	9.0	15	36
Manifold, Head Mount	26.5	9.0	15	18
Other options available. See Ordering Guide, visit www.parrinst.com, or call for more information.				

Operating Modes

The Series 5000 Multiple Reaction System provides an apparatus for running up to six reactions in parallel to build a database for comparing and optimizing operating conditions. The user can design experiments to:

- Run all reactions at the same temperature and pressure while varying catalyst loading or reactant concentrations to optimize these parameters.
- Run all reactors with identical loads varying pressures at a common temperature to study the effect of pressure on reaction rates.
- Run individual reactors with individual loading and temperature and pressure to screen multiple options for activity.

A comparison of the plots of pressure drop versus time within the reactors running under parallel conditions will usually be the most useful means of measuring reaction rates and comparing operating conditions. The internal thermocouple also provides a means of detecting temperature changes due to exothermic reactions.

Reactor Options

As Parr customers have come to expect with our line of laboratory pressure reactor equipment, these reactors are offered with a number of options which permit the user to configure the system to their reactions and intended operating conditions. These options include:

O-ring or Flat Gasket Seals. Vessels with O-ring seals are closed by simply tightening the screw cap down hand tight. The maximum operating temperature will depend upon the O-ring material. When equipped with FKM (Viton®) O-rings operating temperatures up to 225 °C are permitted. By substituting FFKM (Kalrez®) O-rings this limit can be raised to 300 °C. Careful consideration of chemical compatibility must also be given when selecting O-ring materials. PTFE gaskets can be used to temperatures up to 300 °C and offer virtually universal chemical compatibility. Six compression bolts are used to develop the sealing forces on the PTFE gaskets in this design.

5000 Multiple Reactor System (MRS)

MRS with individually controlled Gas Burettes.

Head Configuration. Each reaction vessel is equipped with an inlet valve, exhaust valve, safety rupture disc, and pressure transducer in addition to an internal thermocouple. Vessels can be modified to include a dip tube for liquid sampling or a cold finger for cooling. The user can choose to have the valves, transducer and rupture disc mounted on a gage block connected directly to the vessel head, or remotely mounted on the back panel.

- **Head Mounted.** The head mounted design makes it possible to remove the pressurized vessels from the heater/stirrer assembly or to prefill the vessels in a remote location. PEEK flexible tubing with a quick slip connector is provided for each vessel for inlet of gas. Tubing is easily removed after gas fill.
- **Panel Mounted.** The remote panel mounted arrangement connects all the pressure inlets/outlets to each vessel with a single PTFE lined stainless tubing. Alternate stainless steel tubing is offered if required. In the panel mount valve configuration the gas inlet tubing generally remains attached to the vessels during operation.

Materials of Construction. Type 316 Stainless Steel is the standard material of construction for both the vessel with its wetted parts and the gage block assemblies exposed to vapors. For investigators working with systems containing strong mineral acids or other more corrosive systems these vessels can be made of most of the Parr standard materials of construction.

Stirrer Configuration. Stirring is accomplished by use of either PTFE coated or glass coated magnetic stirrer bars.

Thermocouple Configuration. Thermocouples are mounted inside the vessel for the best temperature monitoring and control. The thermocouples are protected by stainless steel sheaths which are inserted into a protective thermowell. These thermowells make it easy to install and remove thermocouples from the vessels, and also provide additional chemical and mechanical protection for the thermocouple.

We also offer an external thermocouple option with the thermocouples positioned in contact with each cylinder wall.

Gas Manifold. The brass gas inlet manifold is designed to handle both a purge gas, usually nitrogen, and a reactant gas, usually hydrogen. This can be set up to automatically fill each vessel to the same initial pressure or to manually fill each vessel to a unique operating pressure. This gas manifold can also be supplied in T316SS to meet more corrosive requirements.

4871 Process Controller

The Series 5000 Multiple Reaction System is controlled by a dedicated Parr 4871 Process Controller. A detailed description of this controller is found in Chapter 4 of this catalog, pages 95-100.

For this application the controller is set up to provide:

- Temperature monitoring and PID control of each individual reactor.
- Pressure monitoring of each individual reactor.
- Data logging of temperature and pressure in each reactor.
- Control and logging of the common stirring speed of the reactors.

The controller provides Ramp & Soak programming for individual reaction vessels, digital inputs and outputs for interlocks, alarms or other safety features, and additional analog and digital inputs and outputs to control flow meters or other accessories which might be added at some future date. The user's control station is a PC running any current Windows operating system. A simplified graphical user interface has been designed for the control and monitoring of the Series 5000 Multiple Reaction System. The PC is used strictly as the user interface and data logging module. All control actions are generated in the 4871 Process Controller (not the PC).

5000 Ordering Guide

The Order No. for the Base System is: **5000(45)-T-SS-115-P-MV-2000-MB-CC**

A composite identification number to be used when ordering a 5000 Series Reactor can be developed by combining individual symbols from the separate sections below. For more information on how to use this ordering guide, please see page 27.

A Base Model

Model No.	Size
5000	45 or 75 mL

B Gasket / Maximum Temperature

-OV	FKM O-ring, 225 °C
-OK	FFKM O-ring, 300 °C
-T	PTFE Flat Gasket, 300 °C

C Materials of Construction

-SS	T316 Stainless Steel
-MO	Alloy 400
-IN	Alloy 600
-HB	Alloy B-2 / B-3
-HC	Alloy C-276
-CS	Alloy 20
-TI2	Titanium Grade 2
-TI4	Titanium Grade 4
-ZR702	Zirconium Grade 702
-ZR705	Zirconium Grade 705

See page 11 for complete list of available alloys.

D Electrical Supply

-115	115 VAC
-230	230 VAC

E Thermocouple

-No Symbol	Type J (Standard)
-K	Type K

F Valve Mounting

-H	Head Mount w/ PEEK Tubing
-P	Remote Panel Mount w/ PTFE Lined SS Hoses

G Inlet Valve

-AC	Automatic Check Valve
-MV	Manual Valve

H Transducer Range

-1000	0-1000 psi
-2000	0-2000 psi
-3000	0-3000 psi

I Stirrer Type

-MB	Magnetic Bar Stirrer, PTFE
-GB	Magnetic Bar Stirrer, Glass

J Stirring Control

-M	Manual
-CC	Computer Controlled
-RPM	Digital RPM Display

K Certifications

-No Symbol	No Certification
-ASME	ASME Certification
-PED	PED Certification
-CH	China Certification
-P	Parr Certification

L Options

-SV*	Dip Tube with Sampling Valve
-CF*	Cold Finger
-MPG	Manifold Pressure Gage
-FMH	Flexible SS Hoses
-E-TC	External Thermocouple
-R-TC	Redundant Thermocouple
-RCS	Reactor Cooling Support

* Dip Tubes & Cold Fingers cannot be installed at the same time.

Other Available Options

Glass Liner
PTFE Liner

M Spare Parts Kit

-5009	Spare Parts Kit for 5000 Series

Combinatory Chemistry & High-Throughput Screening

Parr designs and builds custom multiple reactor systems for use in combinatorial chemistry and high-throughput screening. These systems are based on our wide range of reactor systems and feature overhead magnetic drive stirrers. Contact our Customer Service Department for details and proposals for custom multiple reactor systems.

Five Reactor Parallel System

This Parallel Reactor System incorporates five 160 mL, 4560 Series Stirred Mini Reactors rated for use at 350 °C and 3000 psig / 200 bar. Each of the reactors has a dedicated high pressure (5000 psig / 345 bar) 100 mL general purpose vessel associated with it serving as a reactant gas feed reservoir. These feed vessels are located above and immediately behind the main reactors and are each equipped with a dedicated pressure transducer, thermocouple and a constant pressure regulator. The regulator maintains the downstream reactor at a constant pressure while the pressure transducer/thermocouple combination allows the process controller to accurately monitor and record the real-time consumption of reactant gas. This system would normally be used to study various aspects of hydrogenation or carbonylation reactions. The 4871 Process Controller also controls and records the reactor temperature, stirring speed and monitors the reaction pressure. The compact reactor system stand incorporates not only reactant gas feed and vent/ purge manifolds but cooling water feed and drain manifolds to simplify the installation and hook up.

16 Station Multiple Reactor System

This system is a combination of sixteen standard 4560 Mini Reactors with heaters, valves, pressure gages and rupture disc assemblies and two 4871 Process Controllers with sixteen 4875 Power Controllers. It allows the user to run multiple reactions simultaneously, applying the principles of high-throughput experimentation. Individual variables that can be controlled are gas mixtures, liquids, catalysts or other solids, stirring speed, temperature, pressure and time.

12 Station HPCL System

This system makes use of the lower cost 5500 High Pressure Compact Lab Reactors that feature a modified stand, aluminum block heaters, removable vessels and a standard gage block assembly. A control system (not pictured) automates the process, monitors the parameters and collects the data.

Three Reactor Parallel System

This system incorporates three 1.8 L 4570 Series High Pressure/ High Temperature reactors rated for use at 5000 psi (345 bar) @ 500 °C. The reactors in this system are manufacatured of Alloy C-276 and are equipped with internal coupon holders to facilitate study of corrosion processes in harsh environments. This application does not require precisely controlled gas delivery; hence individual gas feed vessels are not present, though gas supply and gas vent manifolds are provided. A 4871 Process Controller is also included (not shown).

Four Reactor Parallel System

This system consists of three 160 mL and one 450 mL 4560 Series Reactors rated for use at 3000 psi (200 bar) @ 350 °C. This configuration allows both high throughput screening and scale-up, if desired. Gas supply and vent manifolds for the entire system and pressure control for the larger reactor are provided. Reactor temperatures and stirring speed are controlled by four 4848 Reactor controllers (not shown).

Six Reactor Parallel System with Automatic Sampling System

This system includes six 25 mL, 4590 Series Stirred Micro Reactors rated for use up to 3000psi (200 bar) @ 350 °C. Gas supply and vent manifolds are provided, as well as manifolds to deliver and drain cooling water to/from either the internal cold finger or the external aluminum block heaters with cooling channels. Note the automated liquid sampling system present on the reactor on the left. This sampling system allows the sequential collection of several ~1 mL liquid samples under full reactor operating pressure, and automatically clears the liquid sampling lines between samples. Control is provided by a 4871 Process Controller.

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