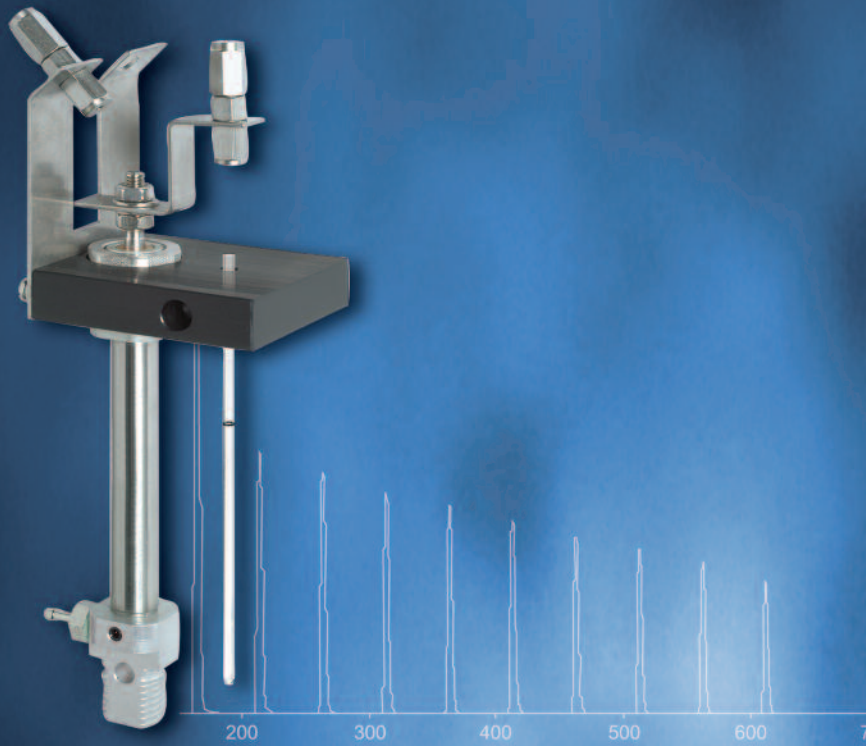


## Thermo Scientific GasBench II



*The Universal On-Line Gas Preparation and  
Introduction System for Isotope Ratio MS*

## The Universal On-Line Gas Preparation and Introduction System for Isotope Ratio MS

The Thermo Scientific GasBench II is an innovative solution for high precision on-line isotope and molecular ratio determination of headspace samples, including water equilibration, carbonates, and atmospheric gases (e.g. CO<sub>2</sub>, O<sub>2</sub>/N<sub>2</sub>). The precision and accuracy of the dual viscous flow inlet system are achieved using modern “continuous flow” techniques.

The GasBench II is not only an alternative to dual inlet system techniques but it significantly extends the practice of isotope ratio mass spectrometry (IRMS).

- Multiple loop injection leads to high precision
- Automation leads to high sample throughput
- High sensitivity results in low sample consumption
- GC separation delivers pure analyte from gas mixtures
- Automatic range recognition and autodilution leads to the largest dynamic range of sample size
- Extreme flexibility leads to very high versatility



Thermo Scientific GasBench II  
On-Line Gas Preparation  
Multiple Loop Injection

# Application Overview

## The Range of Applications Includes, but is not Limited to:

- D/H in water through equilibration with  $\text{H}_2/\text{Pt}$
- $^{18}\text{O}/^{16}\text{O}$  in water through equilibration with  $\text{CO}_2$
- $^{18}\text{O}/^{16}\text{O}$  and  $^{13}\text{C}/^{12}\text{C}$  from carbonates
- $^{13}\text{C}/^{12}\text{C}$  of dissolved inorganic carbon (DIC)
- $^{13}\text{C}/^{12}\text{C}$  and  $^{18}\text{O}/^{16}\text{O}$  of  $\text{CO}_2$  in air
- $^{18}\text{O}/^{16}\text{O}$  and  $^{17}\text{O}/^{16}\text{O}$  of  $\text{O}_2$  in air and water
- $^{15}\text{N}/^{14}\text{N}$  of  $\text{N}_2$  in air

## In Combination with the PostCon Cryotrapping Options or the PreCon:

- $^{13}\text{C}/^{12}\text{C}$  of  $\text{CO}_2$  in air (sub-ambient concentrations)
- $^{15}\text{N}/^{14}\text{N}$  and  $^{18}\text{O}/^{16}\text{O}$  of  $\text{N}_2\text{O}$  in air (300 ppb)
- $^{13}\text{C}/^{12}\text{C}$  of  $\text{CH}_4$  in air (1.7 ppm)
- $^{15}\text{N}/^{14}\text{N}$  and  $^{18}\text{O}/^{16}\text{O}$  of  $\text{N}_2\text{O}$
- $^{15}\text{N}/^{14}\text{N}$  and  $^{18}\text{O}/^{16}\text{O}$  of nitrate using the Sigman technique
- $^{15}\text{N}/^{14}\text{N}$  of  $\text{N}_2$  from micro-preparation systems

## Flexible Design Allows use with Lasers and Elemental Analyzers

- Sampling of  $\text{CO}_2$  and  $\text{SO}_2$  from laser combustions and decarbonation
- Post-combustion concentration of  $\text{CO}_2$ ,  $\text{N}_2$ ,  $\text{SO}_2$  from elemental analyzers

Due to the versatility of the GasBench II the list of gas species, isotope ratios, and experiments that can be performed with the GasBench II is constantly being extended.

## Wide Range of Applications



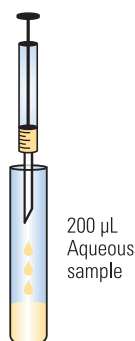
## GasBench II Applications

### $\text{H}_2/\text{H}_2\text{O}$ and $\text{CO}_2/\text{H}_2\text{O}$ Equilibration for $\delta\text{D}$ and $\delta^{18}\text{O}$ Determination of Water

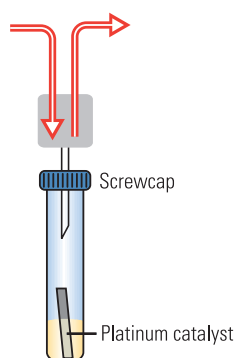
The measurement of the D/H and  $^{18}\text{O}/^{16}\text{O}$  ratios of water is one of the most important applications of isotope ratio mass spectrometry. There is a very diverse range of applications ranging from studies of variations in natural isotope abundance in the hydrologic cycle, to authenticity control on beverages, to metabolic studies using D- or  $^{18}\text{O}$ -enriched tracers in humans and animals. This extreme range of sample types demands a flexible general purpose analytical solution, which can provide high precision / high accuracy / high throughput analysis of  $^{18}\text{O}/^{16}\text{O}$  and D/H.

The aqueous samples are placed in 10 ml screw top vials using disposable pipettes. For D/H, a platinum catalyst is added. The vials are sealed with septa and all air is removed from the sample vials by an automated, autosampler-assisted flushing procedure which uses a mixture of either  $\text{H}_2$  or  $\text{CO}_2$  in He. The  $\text{H}_2$  or  $\text{CO}_2$  in the flushing He stream is used as equilibration gas. After the required equilibration time (D: 40 min,  $^{18}\text{O}$ : 20 h) the whole batch of samples is analyzed. The use of repetitive loop injection (1-2 min per replicate) achieves analytical precisions comparable to those from a dual inlet system.

Alternatively, the TC/EA, the quantitative high temperature carbon reduction Elemental Analyzer, can be integrated with the GasBench II for high precision analysis of D/H and  $^{18}\text{O}$  from a single sub- $\mu\text{L}$  injection of water.

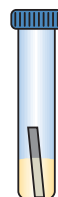


- Place 200  $\mu\text{L}$  of the sample in the vial

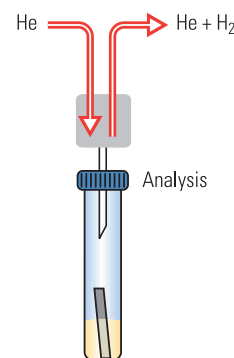


- Place all sample vials in the autosampler tray
- All vials are automatically flushed

D transfer from  
 $\text{H}_2\text{O}$  into  $\text{H}_2$  in  
the headspace



- Equilibrate for 40 min



- Start the Sequence Acquisition

### Dissolved Inorganic Carbon

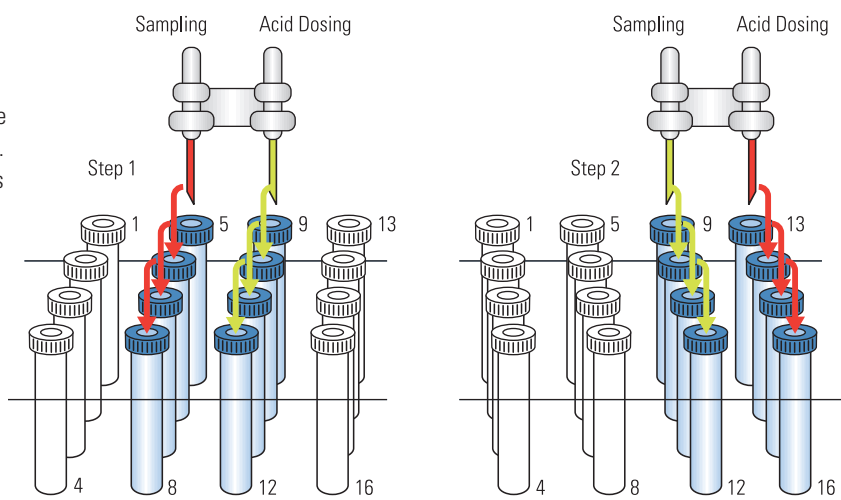
A request to replace the laborious manual preparation of  $^{13}\text{C}$  of DIC for dual inlet analysis with a fast, reliable and accurate continuous flow method is, in fact, what led to the development of the GasBench II. The requirement of  $< 0.1\text{‰}$  precision was readily exceeded, with precisions of  $0.03 - 0.05\text{‰}$  being shown by users. It is safe to say that the GasBench II has revolutionized DIC analysis.

The risk of adsorption of  $\text{CO}_2$  from air into the sea water during sample handling requires a different preparation of the sample vials. 3 drops of phosphoric acid (ca.  $3\text{ }\mu\text{L}$ ) are placed in the empty vials. After sealing the vials with septa, all vials are automatically flushed with pure helium. The sea water samples are injected using gastight, disposable syringes.

After a short reaction time, the  $\text{CO}_2$  in the headspace of each vial is automatically analyzed using the same acquisition process as for all other GasBench II applications.

## $\delta^{18}\text{O}$ and $\delta^{13}\text{C}$ Determination of Carbonates

For more than 50 years,  $\delta^{18}\text{O}$  and  $\delta^{13}\text{C}$  measurements of carbonates have been one of the major applications of stable isotopes. The analysis of foraminifera, in particular, is one of the most demanding applications, requiring both high precision and high throughput.



## The Carbonate Reaction Kit

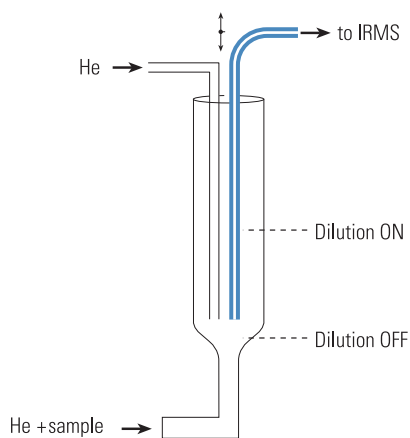
The GasBench II in carbonate mode uses the principle of individual acid baths using a fully automated acid dosing system. The carbonate option contains a microliter pump that allows injection of anhydrous phosphoric acid (103%) into the sample vials. The double needle setup ensures identical reaction and analysis conditions for each sample. Laboratories have shown that 80 samples per day (including 14 standards for quality control) can be processed in routine operation. An overall precision of 0.08 ‰ for  $\delta^{18}\text{O}$  and of 0.06 ‰ for  $\delta^{13}\text{C}$  has been achieved.

## The Autodiluter

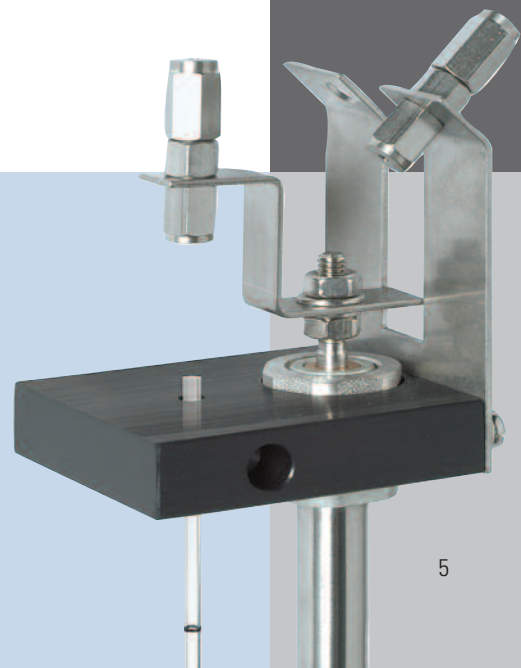
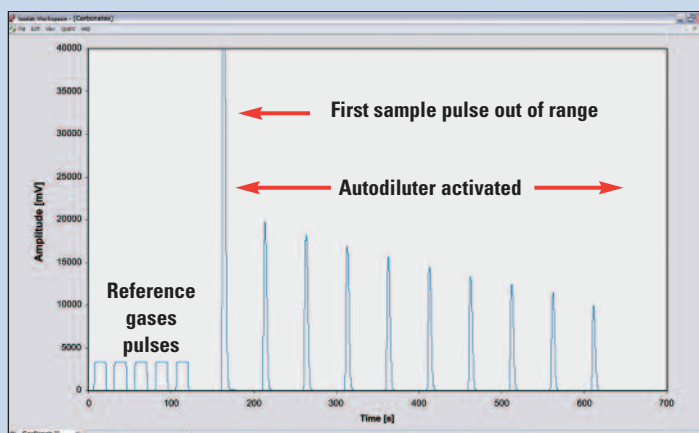
The GasBench II offers a unique computer-controlled Autodiluter capability. If the signal height of the first sample peak exceeds a pre-defined threshold (e.g. 20 V), the diluter is activated resulting in a 3-fold reduction in signal height for the subsequent sample peaks. The dilution is performed in the open split, just before transfer into the ion source, eliminating any possible effects on the integrity of the sample gas.

The Autodiluter capability allows analysis of samples that would normally be too large to be measured. This capability offers clear advantages in sample preparation, because it reduces the need for time-consuming weighing of samples, and it allows analysis of samples with unknown amounts of carbonates (e.g. whole rock samples with carbonate cements).

## Principle of the Autodiluter



## Thermo Scientific GasBench II Data Acquisition, 10 Sample Pulses, Autodiluter Activated by First Sample Pulse



## Technical Details

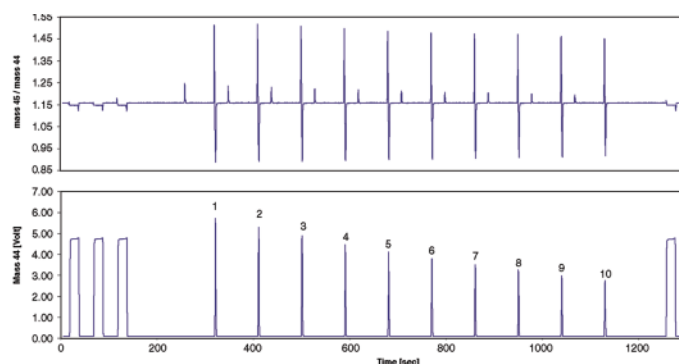
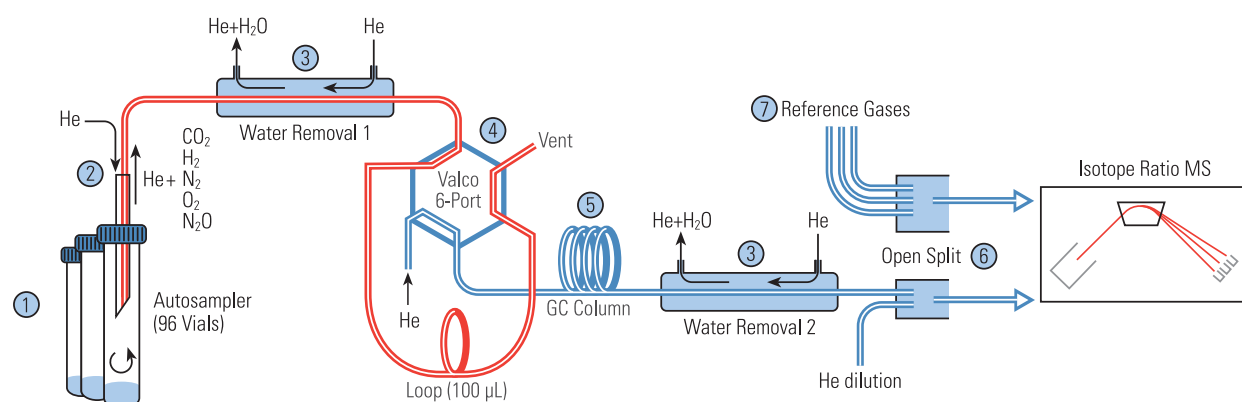
The GasBench II consists of a user-programmable autosampler (1), a gas sampling system (2), a maintenance-free water removal system (3), a loop injection system (4), an isothermal gas chromatograph (GC) (5), an active open split interface (6), a reference gas injection system with three reference ports (7), and one or two optional LN2 traps for cryofocusing.

The autosampler can be equipped with a variety of sample trays. A precisely thermostated sample tray is used for carbonates and water equilibration.

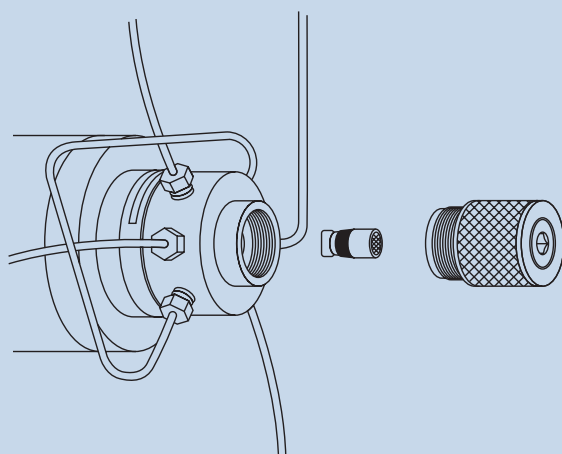
The gas sampling system includes a two port needle which adds a gentle flow of He into the sample vial, thus diluting and displacing sample gas. Water is removed from the sample gas through diffusion traps. The loop injector aliquots the sample gas onto the GC column, which separates the molecular species. The reference gas injection system allows accurate referencing of each sample aliquot to isotopic standards. The system is designed for unattended measurements with high throughput, ensuring high productivity and high reliability.

The GasBench II can be used for the isotopic characterization of  $\text{CO}_2$ ,  $\text{N}_2\text{O}$ ,  $\text{O}_2$  or  $\text{N}_2$  between 200 nmol and 20  $\mu\text{mol}$  of total sample size. The  $\text{CO}_2$  can be in the original gas sample (air or breath), be released through a preparation step (carbonates, DIC) or be added to the original liquid sample (water- $\text{CO}_2$  equilibration).

### GasBench Scheme



Single sample acquisition with 10 replicates



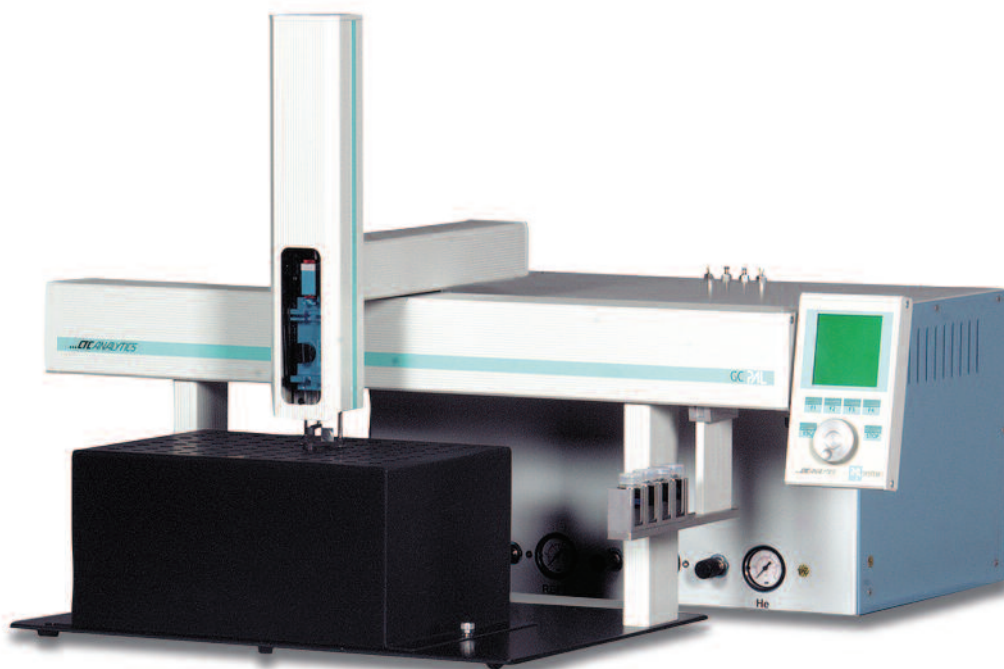
# The GasBench Principle

The GasBench II allows the precision and accuracy of the dual inlet system to be realized on a CF-IRMS system. The dual inlet principle of repetitive measurements of sample and standard gas is not only retained, it is generalized. The sample volume is the sample vial (instead of a metal bellows), and the reference gas volume is a pressurized gas tank. Reference gas pulses are introduced under computer

control into to the carrier gas stream from the reference injection system.

The sample gas is entrained in He, which allows GC separation and facilitates fractionation-free viscous flow transport of the sample aliquots. In a typical experiment, ten aliquots of the sample will be taken from the sample vial, dried and cleaned on-line, and measured against reference gas pulses. The sample consumption is much

lower than for the dual inlet system, while comparable precisions are achieved, including an analysis of internal reproducibility.

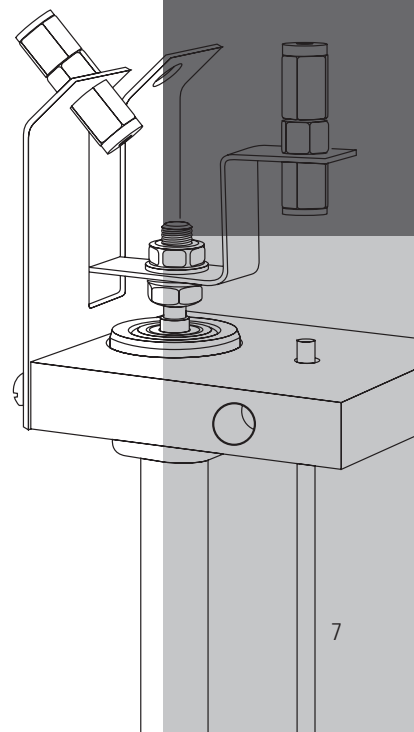


**The combination of “Repetitive Loop Injection” and Reference Gas Injection is a generalization of the analytical procedure of sample-standard comparisons performed with a dual viscous flow inlet system.**

## Comparison to the “Classical” Dual Inlet System

During a dual inlet measurement, sample and reference gases confined in variable volumes close to the ion source are sampled alternately and repeatedly through a changeover valve. This measurement strategy leads to high analytical precision and accuracy. Internal reproducibility of the

individual measurements is a commonly used measure of analytical quality which, up to now, has been missing from CF-IRMS inlet systems. The drawbacks of the dual inlet system include off-line sample preparation and purification, ineffective use of the sample gas, lengthy data acquisitions, and cost.

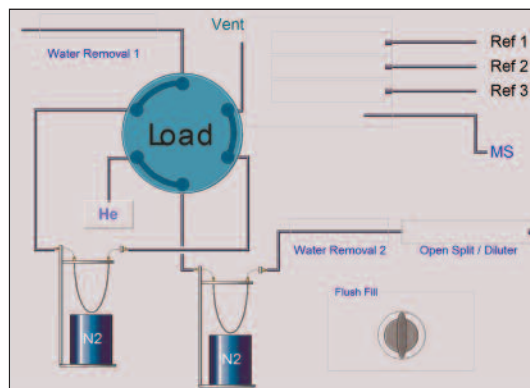




## GasBench II Options

- Carbonate Reaction Kit  
The carbonate option contains a micro-liter pump that allows injection of anhydrous phosphoric acid (103%) into the sample vials and a dual needle array for dosing and sampling
- 96 Sample tray (ambient temperature)
- 96 Sample tray (temperature controlled)
- Single cryotrap  
Trapping option with a single fused silica trap for sub ambient gas concentration (e.g. 100 ppm CO<sub>2</sub>)
- Dual cryotrap (PostCon)  
Trapping option with two traps, one 1/16" nickel-wire filled stainless steel trap for trapping ppm amounts of analyte from a fast He gas stream, and one fused silica trap for cryo-focusing onto the GC column head

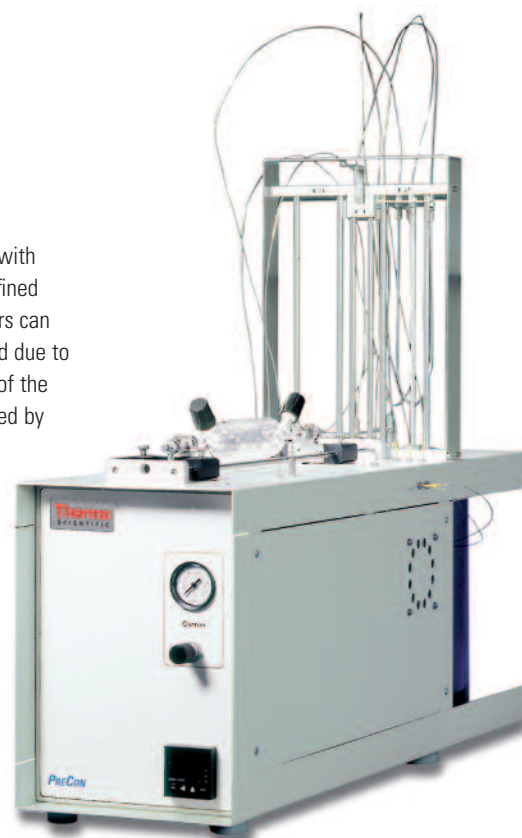
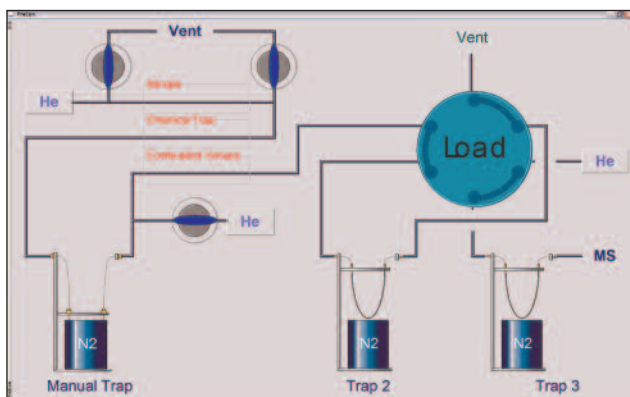
- Autosampler extensions  
The GasBench II autosampler can be extended to automate a second peripheral device, including the TC/EA, EA, H/Device, and PreCon.



## PreCon Integration and Automation

For gas concentrations in the low ppm and ppb range, the PreCon gives access to the fully automated preparation and pre-concentration of trace gases such as N<sub>2</sub>O (300 ppb) and CH<sub>4</sub> (1.7 ppm) followed by cryogenic focusing in front of the GC column. The PreCon can be loaded manually or operated fully automatically using the GC-PAL autosampler of the GasBench II with the two line needle for continuous sample transfer.

The GC-PAL can be equipped with a 96 x 12 mL sample tray. User-defined sample trays and sample containers can easily be registered and automated due to the fully object oriented structure of the GC-PAL. All processes are controlled by user-definable Isodat 2.0 scripts.



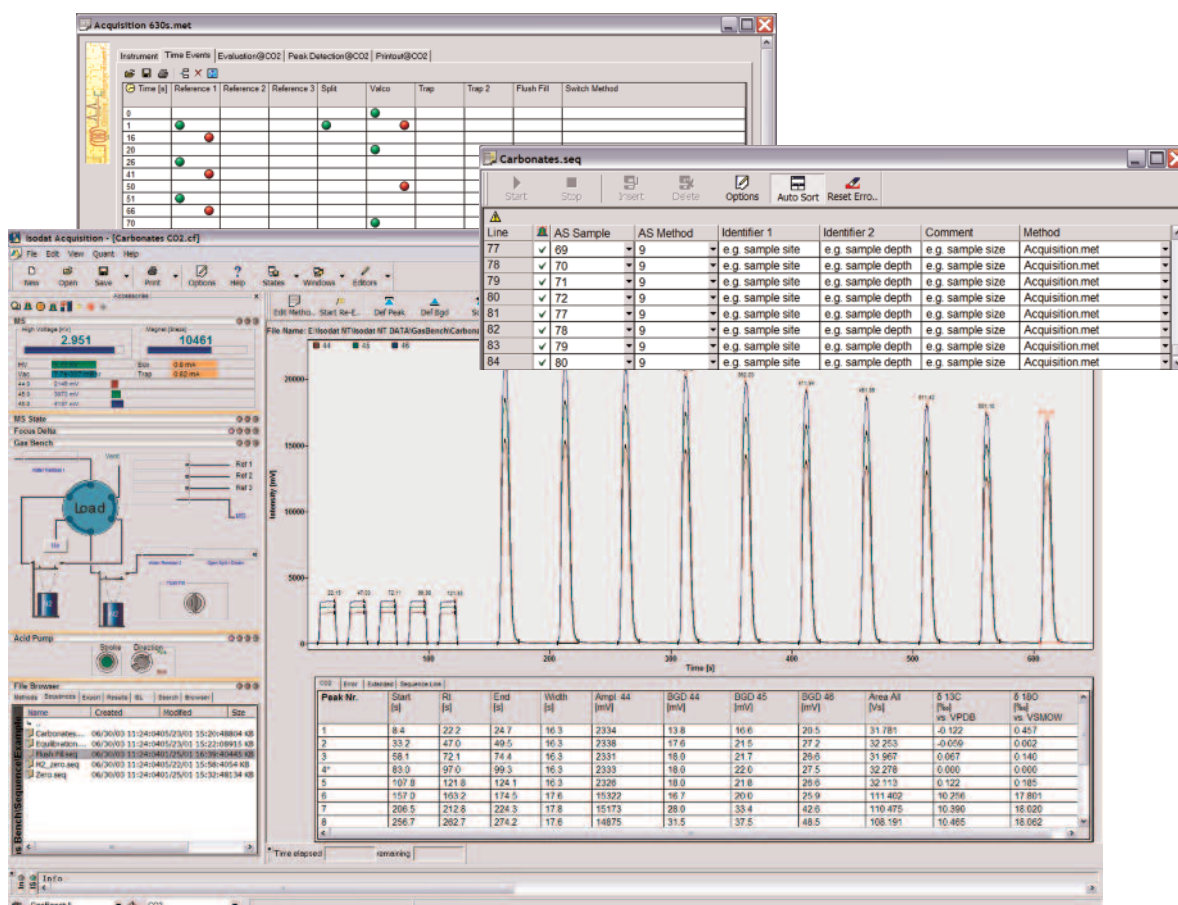


# Thermo Scientific Isodat Software Suite

The Isodat software suite is the software suite for system control, data acquisition and data evaluation. The advantage that the Isodat software suite offers for GasBench II applications include:

- Easy and fast method and sequence setup for IRMS, GasBench II preparation and acquisition modes.
- Complete control and automation of all interface functions for sample preparation and data acquisition.
- Automated peak and background detection with a wide selection of dedicated detection and background subtraction algorithms.
- Fully automated correction of the GC elution time shift of isotopomers.
- Fully automated  $H_3^+$  correction of each single raw data point.
- Fully automated ion correction for isobaric ion contributions such as  $^{12}C^{17}O^{16}O$  on  $^{13}C^{16}O^{16}O$ .
- User defined ion correction formulas can be registered in the Isodat software suite using the Isodat Script Language (ISL).
- Full access to all raw data and processed data.
- Full access to ion correction algorithms and intermediate data.
- Access to easy batch reprocessing, manual peak and background definition including printouts and data export.
- Fully customizable and multiple exports of evaluated data to Excel, other spreadsheet programs and databases (LIMS).
- All printouts are fully customizable due to object oriented print-out templates using the unique Isodat Result Workshop package.
- Full network compatibility with direct and fast access to Windows tools.
- Complete Isodat system backup and retrieval within minutes using the Isodat Version Handler.

Based on the unique "Plug and Measure" concept of the new generation of IRMS (DELTA<sup>plus</sup> XP, DELTA<sup>plus</sup> Advantage and MAT 253), the GasBench II interface and preparation unit is immediately recognized and operational.



## Analytical Performance

For Thermo Scientific DELTA Series or MAT 253 Mass Spectrometers

### Thermo Scientific GasBench II Basic Performance

#### 10 pulses of reference gas (amplitude 3V, H<sub>2</sub> 5V), $\delta$ notation

		Precision (1 $\sigma$ )	Linearity
CO <sub>2</sub>	<sup>13</sup> C	0.06 ‰	0.02 ‰/nA
CO <sub>2</sub>	<sup>18</sup> O	0.08 ‰	0.02 ‰/nA
O <sub>2</sub>	<sup>18</sup> O	0.08 ‰	0.02 ‰/nA
N <sub>2</sub>	<sup>15</sup> N	0.06 ‰	0.02 ‰/nA
H <sub>2</sub>	<sup>2</sup> H	0.50 ‰	0.20 ‰/nA

An ion current range of 2 – 20 nA (0.6 – 6 V) is equivalent to 1.2 µg – 12 µg carbon equivalent in the headspace of a 12 mL vial

### External Precision of Isotope Ratios C, O, H, using the Thermo Scientific GasBench II with 12 mL Vials (n=5), $\delta$ Notation

#### Water equilibration (versus V-SMOW & SLAP)<sup>(1)</sup>

500 µl	as CO <sub>2</sub>	$\delta^{18}\text{O}$	< 0.08 ‰
200 µl	as H <sub>2</sub>	$\delta^2\text{H}$	< 2.0 ‰
		$\delta^2\text{H}$	< 0.5 ‰ on raw data <sup>(1)</sup>

#### Carbonates

100 µg	as CO <sub>2</sub>	$\delta^{18}\text{O}$	< 0.1 ‰
		$\delta^{13}\text{C}$	< 0.1 ‰

#### Dissolved inorganic carbon, ocean water

600 µl	as CO <sub>2</sub>	$\delta^{13}\text{C}$	< 0.08 ‰
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#### CO<sub>2</sub> in air

12 ml	as CO <sub>2</sub>	$\delta^{13}\text{C}$	< 0.2 ‰
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<sup>(1)</sup> V-SMOW & SLAP scaling: Based on IAEA recommendations all <sup>18</sup>O and D analysis need to be based on V-SMOW and SLAP.

For H<sub>2</sub>/H<sub>2</sub>O equilibration with platinum catalyst, this referencing results in a scale expansion of up to 4 times from the raw delta values to the final data, which equivalently decreases the precision of measurements.

On <sup>18</sup>O determinations (CO<sub>2</sub>/H<sub>2</sub>O) this data processing also needs to be performed but the scaling factor usually is almost 1 and therefore has no effect on the performance data.

### Acceptance Specification

During installation, the system performance of the GasBench II will be demonstrated with a mixture of CO<sub>2</sub> in He ( $\geq 0.3\%$ ), to show an external precision of 0.08 ‰ for  $\delta^{13}\text{C}$  and  $\delta^{18}\text{O}$  (n=5).

A mixture of H<sub>2</sub> in He mixture ( $\geq 1.0\%$ ) is used to show an external precision (n=5) of 2.0 ‰ for  $\delta^2\text{H}$ .



# Installation Requirement

## Power

230 V single phase, 8 A

## Gases

- He, better 99.999%
- CO<sub>2</sub>, better 99.995%
- H<sub>2</sub>, better 99.999%
- 0.3% - 1% CO<sub>2</sub>, (99.995%) in He (99.999%) for <sup>18</sup>O water equilibration
- 1.0% - 2.0% H<sub>2</sub> (99.999%) in He (99.999%) for <sup>2</sup>H water equilibration

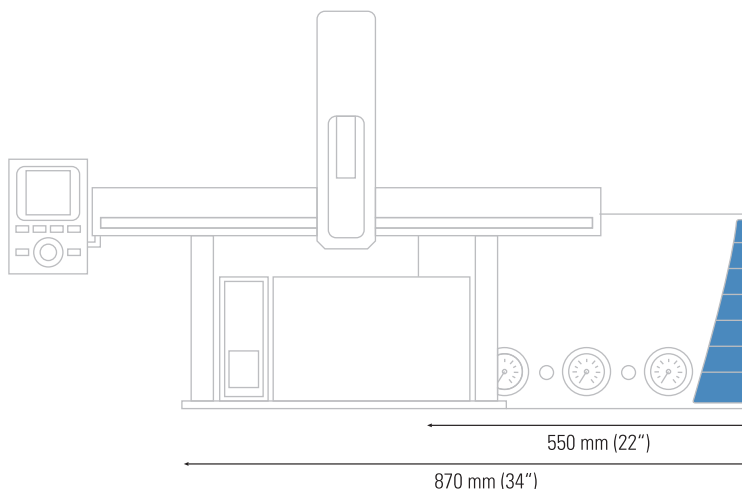
## Weight

- GasBench II 14 kg
- Heated tray, GC Pal, and Baseplate 43 kg

## Optional items

- PoraPLOT Q capillary column for separation of N<sub>2</sub> and CO<sub>2</sub> (included in the standard GasBench II system)
- Carbonate kit with dual needle support, acid pump and needle, phosphoric acid for carbonate analysis
- Temperature stabilized tray with 96 x 12 mL vials for carbonate and water analysis
- Hydrophobic Pt catalyst sticks for H<sub>2</sub>/H<sub>2</sub>O equilibration
- 5Å PLOT capillary column for good chromatographic resolution and thus high precision isotopic measurements of the molecular components of air (N<sub>2</sub>, O<sub>2</sub>, Ar, CH<sub>4</sub>, CO)
- Single cryo trap for trapping of trace gases from low He flow systems
- PostCon dual cold trap for trapping of trace gases from high He flow systems with subsequent cryofocusing in the second trap

## GasBench II Footprint and Dimensions



## Literature

- A simple, practical methodology for routine VSMOW/SLAP normalization of water samples analyzed by continuous flow methods, S.T. Nelson, Rapid Commun. Mass Spectrom. 14, 1044–1046 (2000)
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- A bacterial method for the measurement of the oxygen isotopic composition of nitrate in marine and fresh waters, K.L. Casciotti, D.M. Sigman, M.G. Hastings, J.K. Böhlke, and A. Hilkert, Analytical Chemistry, 74, 4905–4912 (2002)
- Using septum-capped vials with continuous-flow isotope ratio mass spectrometric analysis of atmospheric CO<sub>2</sub> for Keeling plot applications, K.P. Tu, P.D. Brooks and T.E. Dawson, Rapid Commun. Mass Spectrom. 15, 952–956 (2001)

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