

# WS-CRDS for Isotopes – Cost of Measurement Comparison with IRMS for Liquid Water

**Summary.** Picarro WS-CRDS isotopic analyzers offer significantly lower capital costs than traditional isotope ratio mass spectrometry (IRMS) instruments. There is also a dramatic difference in the operating costs of the two technologies, making WS-CRDS a very attractive option.

## Introduction

Picarro WS-CRDS based isotopic analyzers offer numerous advantages over traditional isotope ratio mass spectrometry (IRMS) instruments, while providing similar or better performance. These advantages include transportability, ruggedness and incredible simplicity of operation. One of the biggest and most dramatic advantages is cost of ownership, i.e. cost of measurement. In this whitepaper we provide a detailed breakdown and analysis of the complete cost of owning and operating both instrument types when used to obtain  $\delta^{18}\text{O}$  and  $\delta\text{D}$  for liquid water samples. We show that the capital costs are a factor of *four* lower for WS-CRDS and operating costs are a factor of *three* lower for WS-CRDS compared to a temperature conversion/elemental analyzer (TC/EA IRMS) system. Further, the need to have professionally trained operators for IRMS systems adds another approx. \$115,000 per year to the budget for those systems which is not required for WS-CRDS. Overall, investing in a low-cost WS-CRDS instrument can significantly reduce overall laboratory expenditure, or increase throughput through the acquisition of multiple analyzers.

## Summary of Primary WS-CRDS Advantages

Before providing a detailed running cost comparison, it is useful to compare these two competing isotopic analysis technologies.

A major difference is in size and weight. Whereas an IRMS system is about the size of a small desk, a WS-CRDS instrument is roughly the size of a briefcase (see Figure 1). Even when configured for automatic handling of multiple liquid samples, the WS-CRDS is still a small benchtop instrument. In addition to the savings in valuable laboratory space, the low weight and size of WS-CRDS technology means these instruments are fully transportable allowing them to be used as a shared resource. Moreover, in combination with their rugged construction, WS-CRDS can be used in unattended field studies and even operated on a moving platform such as a boat, truck or plane. The ability to take the WS-CRDS instrument to a measurement site and even leave it there, reduces the cost, time and risk of spoiling of a captured samples approach and also enables continuous live-stream monitoring. In contrast, IRMS is strictly a stationary lab-bound technology.



*Figure 1. Picarro WS-CRDS instruments have a compact footprint, are transportable and installed in minutes.*

The WS-CRDS also records  $\delta^{18}\text{O}$  and  $\delta\text{D}$  truly simultaneously, both measurements are collected at the same time by the same process. Further, these instruments are far less prone to drift than an IRMS. With IRMS it is necessary and standard practice to alternate samples with reference standards in a data run. So at least half the time, the instrument is running standards rather than unknowns.

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In terms of performance, the WS-CRDS and IRMS are remarkably similar. For example, in the case of  $\delta^{13}\text{C}$ , the WS-CRDS offers typical precision of 0.2‰ to 0.3‰. In the case of liquid water, the particular subject of this cost comparison, typical performance is  $\delta^{18}\text{O} < 0.07\text{‰}$  and  $\delta\text{D} < 0.2\text{‰}$ . With this level of performance, precision should not be a determining factor in the decision to choose IRMS or to replace IRMS with WS-CRDS.

## **Operator Costs**

WS-CRDS instruments are also much simpler to operate than IRMS, offering two key benefits. First, operating an IRMS requires an experienced and skilled operator with extensive training. In contrast, a WS-CRDS can be operated within minutes of opening the shipping package – it really is that automated and that simple. Second, there is the issue of optimized performance. The precision of an IRMS is very dependent on the level of operator skill. This is why a few leading isotope laboratories can sometimes achieve precision that is an order of magnitude higher than an “average” user. In contrast, the WS-CRDS is completely automated and eliminates subjectivity. Any operator can exceed the specified minimum performance.

The financial impact for using highly trained specialists is considerable. The total compensation packages for highly skilled practitioners (those typically holding a Ph.D.) are over \$115,000 a year<sup>1</sup>. Institutions using WS-CRDS gain in two ways. Firstly, use of the instrument in a dedicated lab does not need such a highly trained individual (Technicians are paid about 2/3rds that of Ph.D. scientists). Secondly, the instrument can be installed in the wet lab (analogous to the way in which LC-MS systems have migrated from the instrument facility to the wet lab). Any chemist, already employed, can operate the instrument whenever they need an analysis, thereby saving an institution a full salary.

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<sup>1</sup> See, for example, AAPS Salary Survey, AAPS NEWSMAGAZINE January 2005

## Capital Costs and Instrument Depreciation

As shown in Table 1, depending on options, the approximate list price of a Picarro liquid water isotope analyzer is currently around \$80,000 US. In contrast, an IRMS-based setup fully configured to measure both  $\delta D$  and  $\delta^{18}O$  from liquid water would currently cost around \$300,000 US, depending on manufacturer and model.

Assuming a typical 5-year depreciation model and a nominal \$100 US salvage value, the first year depreciation cost for the Picarro instrument is approximately \$22,000, which translates into twelve monthly installments of just over \$1,800. The IRMS setup, with the same nominal \$100 US salvage value, has a first year depreciation cost of nearly \$83,000; with a monthly cost close to \$7,000.

Higher priced capital equipment such as IRMS is often depreciated using a 7-year model. Using the same nominal \$100 for the salvage value, the first year depreciation for IRMS for this time period is nearly \$66,000 with a monthly value of almost \$5,500. The Picarro product has annual and monthly values of only \$17,500 and \$1,460 respectively – again, almost 4 times cheaper than the IRMS.

**Table 1**

### Year 1 Depreciation

Based on double-declining balance method and assuming a \$100 salvage value

Vendor	List Price	Life	Year 1 Dep.
Picarro	\$80,000	5	\$22,039
IRMS	\$300,000	5	\$82,646
Picarro	\$80,000	7	\$17,534
IRMS	\$300,000	7	\$65,755

## Running Costs of WS-CRDS for Liquid Water

Referring to Table 1, the running costs for a liquid water WS-CRDS isotopic analyzer (Picarro L1102-*i* or L1115-*i*) can be divided into two distinct categories, consumables and spare parts. The former are the inevitable and very predictable costs of operating the instrument on real samples. The latter are parts that might conceivably have to be replaced – for these we have taken conservative estimates by assuming the worst-case possible lifetime for each item. Calculations regarding the consumption of consumables and the replacement of spare parts all assume continuous operation, i.e., 52 weeks of operation per year, 24 hours per day. For both instruments, the cost are calculated using a realistic number of 144 sample injections per day, based on an allowance of 10 minutes per sample, for injection, data acquisition, system purging, etc. In fact, WS-CRDS can be run at 360 sample injections per day without significant compromise in performance. The number and type of both consumables and spare parts, and hence the fundamentals of this comparison, are obviously geographically independent and can be used to accurately compute running costs in any local currency. In order to convert these into actual monetary costs for discussion in this whitepaper, we have used typical 2009 United States prices for all line items in US dollars.

Syringes are multi-use devices but have a finite lifetime. In an 8,700 hour year, a conservative consumption estimate is 26 syringes over the year. In terms of sample containers, we have assumed one sample per disposable vial and that six injections per sample is a fair average; in any case the numbers will be identical whether talking about WS-CRDS or IRMS. This corresponds to a total count of 8,736 vials and caps. Evaporator septa and waste port septa are low cost and long-lived items but we nonetheless include both here for completeness. We assume a six times lower number of waste port (versus evaporator) septa are required simply because there are six injections per sample, but only one waste “injection.”

Other consumables are chemical supplies such as reference samples and dry air. With WS-CRDS and TC/EA IRMS, users will calibrate applications specific secondary standards using purchased

absolute reference standards. We assume here, for both instruments, just the cost of the absolute reference standard (that are available for purchase only once per year through the International Atomic Energy Agency - IAEA).

Although the WS-CRDS systems in the field can be operated using Drierite™, the cost of ownership table includes the cost of dry air from a cylinder which is recommended for ultra high precision measurements. The air is needed to carry the water vapor into the WS-CRDS measurement chamber and to flush this chamber between injections. This is a particularly easy and accurate cost to compute. For 6 x 8736 injections over a one year period, the total dry air needed is eight cylinders - each containing 300 cubic feet equivalent volume at one atmosphere.

As shown in Table 1, the total annual cost of all these consumables for the liquid water WS-CRDS instrument is \$6,427 US.

Moving parts have a finite lifetime. But the only moving parts in a WS-CRDS analyzer are the small pumps used to move the water vapor into and out of the optical measurement chamber. Picarro instruments use a highly reliable diaphragm pump, but it would be unfair to assume an indefinite lifetime. We have therefore assumed a very conservative lifetime of 18 months for each pump. While there are no other finite-lifetime components in the WS-CRDS analyzer we have also inserted a cost for replacement of cooling fans for an average representation of any “unexpected” component failures.

The only other component that has to be considered in a cost computation is the particulate filter. The purpose of this filter is to preclude any possibility of dust getting into the chamber which could absorb and/or scatter the laser light and affect the data. In most cases, this filter will have a lifetime of many years, but for “dirty” samples, this could eventually clog and need replacement. For completeness we have therefore assumed a lifetime of 2 years for this filter.

Based on these calculations, the total cost of “spare parts” is \$2,915 per annum. (As can be seen in Table 1, most of this cost is for pump replacement, so typical costs will probably be much lower than this worst case estimate). The total instrument operating costs are thus about \$9,342 US per year.

### **Comparison: Running Costs of TC/EA IRMS**

As with WS-CRDS, we have separated the running costs of TC/EA IRMS into two categories, consumable items and maintenance items, i.e. spare parts. All the costs associated with handling/presenting the liquid water samples are identical for the two instrument types, e.g., 8,736 vials and caps, 130 evaporator septa, and two sets of standards (3x 20 ml) per year. However, TC/EA IRMS has several other consumables, some with significant costs, mainly as a result of the need to extensively process the water samples.

Specifically, the water must first be broken down. Unlike WS-CRDS, water can never be introduced directly into a mass spectrometer chamber. This separation is performed automatically in a TC/EA front end. This contains a pyrolysis furnace operated at about 1,400 °C where water reacts with the surface of a glossy carbon tube packed with glossy carbon chips. Expensive pure silver wool is used as a packing material to prevent the carbon chips from falling out. This material is preferred over glass wool which becomes brittle after prolonged intense heating. The carbon chips increase the overall carbon surface area and slow the inevitable erosion of the carbon tube, which eventually leaks at its hottest point. This tube then requires typically four to five days of downtime to replace. In a worst case, if the carbon has also melted on to the ceramic furnace tube then that has to be replaced too. In addition to the carbon chips, a small amount of nickelized carbon powder is placed at the very center of the furnace. This activated carbon is consumed much more quickly than the carbon chips and is used sparingly because of its higher cost.

In the TC/EA furnace, reaction with carbon at 1,400 °C converts the water vapor into CO and H<sub>2</sub>. These products are then separated in a gas chromatograph (GC), with a molecular sieve column, before entering the mass spec. The magnetic field is then programmed to re-optimize for CO and deuterium/hydrogen prior to each peak arriving. The GC column has to be replaced at least once a year.

Unlike WS-CRDS, a TC/EA IRMS must be continuously calibrated which changes the economics of calibration. The instrument is calibrated with two working gas standards, a mix of C<sup>18</sup>O and C<sup>16</sup>O, and a mix of D/H. These working standards are periodically calibrated in turn against absolute water standards. In most countries, government regulations mandate that the handling of CO must be accompanied by the use of a CO detector for operator safety purposes. So, the operating costs must reflect this as well. In addition to the costs of the carbon tube, carbon chips, nickelized carbon, silver wool, GC column, and working and absolute standards, a TC/EA system also needs helium to act as an inert carrier gas. Total helium consumption is about 12 tanks (300 cubic ft/tank) for a year of continuous 24/7 operation.

As can be seen from the Table 2, the total annual cost for all these consumables for a TC/EA IRMS is in excess of \$15,000 US, which is much higher than for a WS-CRDS.

There are also significant costs associated with maintenance (spare parts) of the mass spectrometer, which is a high-vacuum device. The single biggest cost in this area is for cleaning the ion source. This involves disassembly of the electrodes and spacers, ultrasonic washing of the parts, drying and then reassembly. A highly experienced operator can perform this cleaning, but with an average downtime of about one week. Instead, most users prefer to handle this with a service contract with the TC/EA IRMS manufacturer. Typical costs for this in the US are around \$8,000 per annum. Maintenance of the turbo vacuum pump, which involves replacement of the felts and oil, is less costly, but still involves considerable down time.

The only other expected maintenance item is the filament used to generate electrons. This is made of tungsten coated with thorium to prevent oxidation and has to be changed at least once per year, although we have assumed only once for fairness in this comparison. In addition to the cost of this filament, opening the chamber to replace it requires a new sealing gasket each time. This can be just a copper flange, but is preferably a gold or iridium wire.

The annual average cost of these maintenance items totals just over \$8,700 U.S. So the total running costs for a TC/EA IRMS are over \$24,000 US per year, based on continuous 24/7 operation, close to 3 times that of the WS-CRDS.

There are additional secondary cost savings of WS-CRDS over IRMS, such as electricity costs. While the IRMS is a high-vacuum instrument with a large pump, WS-CRDS instruments operate with a power budget of less than 500 watts. And, should also consider the cost of lab space. The true cost per square meter varies greatly but it is never zero!

### **Service Contract Costs**

A further cost to consider is that of service contracts. These are generally based on a percentage (typically 10%) of the list price of the instrument. So, the annual service contract for an IRMS will be about \$30,000 per year. This value is about 4 times that for the WS-CRDS analyzer. The service contract for an IRMS system is a desirable insurance policy – the likelihood of breakdown due to part wear or user error is significantly increased by the sheer complexity of the instrument.

### **Conclusion**

Adding together the annual capital depreciation and operating costs of a WS-CRDS instrument and comparing to an IRMS instrument provides a stark contrast. An IRMS system can cost \$75,000 more per year than a WS-CRDS analyzer. In other words, institutions can afford close

to 4 times as many WS-CRDS analyzers (equating to 4 times the throughput) for every IRMS unit they purchase. For organizations new to stable isotope analyses the difference escalates to \$175,000 per year due to the need for a skilled operator, equivalent to an additional 6 WS-CRDS systems.

It is also particularly interesting to compare the absolute difference in annual running costs to the capital cost of the equipment. In this case of liquid water analysis, the difference is around \$15,000 US. That means that the entire capital cost of a WS-CRDS can be recovered five years. So a laboratory currently operating a TC/EA IRMS instrument can switch to a WS-CRDS instrument, and the entire capital cost can be recovered in just a few years, simply from reduced running costs, as described in this whitepaper.

A further perspective is that running a sample load of only 36 samples a day, six days a week for 50 weeks a year over 7 years will result in 75,600 total samples. The total capital and operating cost for the same 7 year period is \$147,000. The cost per sample, on this basis, is less than \$2!

Picarro WS-CRDS isotopic analyzers have won several prestigious awards\* and have been selected by leading stable isotope laboratories around the world because they offer a unique combination of performance and simplicity. But in the current economic climate, where every capital equipment expense must be carefully scrutinized, a relatively mundane factor such as the operating costs may turn out to be the determining factor by which technology is adopted.

\*Picarro isotopic analyzers have been selected for several major awards including an R&D 100 award in 2008, the Pittcon Editors' Choice award in 2009, a Frost & Sullivan Innovation Award in 2009 and recognized in the Wall Street Journal Technology Innovation Awards, 2009.

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**Table 2****Picarro's Liquid Analyzer**

Based on one system in 24/7 operation, and assuming that a maximum of 144 injections can be analyzed in a 24 hour period (~10 min/injection)

<b>Consumable items:</b>	<b>Cost/unit</b>	<b>unit</b>	<b>units/year</b>	<b>cost/year</b>
Syringes	\$57	1	26	\$1,498
Vials & Caps <sup>1</sup>	\$35	100	8760	\$3,066
Evaporator septa	\$40	100	131	\$53
Waste port septa	\$10	20	22	\$11
Standards (set of 3, 20ml each) <sup>2</sup>	\$200	1	1	\$200
Dry air cylinder <sup>3</sup>	\$200	1	8	\$1,600
				<b>\$6,427</b>

<b>Analyzer maintenance items:</b>	<b>Cost/unit</b>	<b>unit</b>	<b>units/year</b>	<b>cost/year</b>
Pump (2 per analyzer) <sup>4</sup>	\$2,000	1	1.4	\$2,800
Particulate filter <sup>5</sup>	\$130	1	0.5	\$65
Cooling fans	\$25	1	2	\$50
<b>Total</b>				<b>\$2,915</b>

<b>Total cost, consumables and maintenance items</b>	<b>\$9,542</b>
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1. Assume 1 sample per vial, 6 injections per sample

2. Assume 20ml lasts for 1 year

3. 300 cu ft

4. Assume 18-month lifetime

5. Assume 2-year lifetime

**Table 3****TC/EA-IRMS**

Based on one system in 24/7 operation, and assuming that a maximum of 144 injections can be analyzed in a 24 hour period (~10 min/injection)

<b>Consumable items:</b>	<b>Cost/unit</b>	<b>unit</b>	<b>units/year</b>	<b>cost/year</b>
Syringes	\$57	1	26	\$1,498
Vials & Caps <sup>1</sup>	\$35	100	8760	\$3,066
Evaporator septa	\$40	100	131	\$53
Waste port septa	\$10	20	22	\$11
Standards (set of 3, 20ml each) <sup>2</sup>	\$200	1	1	\$200
Helium gas <sup>3</sup>	\$300	1	12	\$3,600
Glassy carbon tube	\$1,000	1	4	\$4,000
Glassy carbon chip	\$100	1	12	\$1,200
Silver wool	\$65	1	4	\$260
Nickilized carbon	\$50	1	4	\$200
CO std gas tank	\$600	1	1	\$600
GC Column 5A Molsieve	\$250	1	1	\$250
H2 Gas tank	\$200	1	1	\$200
CO gas detctor	\$50	1	NRC	\$50
<b>Total</b>				<b>\$15,187</b>

<b>Analyzer maintenance items:</b>	<b>Cost/unit</b>	<b>unit</b>	<b>units/year</b>	<b>cost/year</b>
Ion source Thermo cleaning <sup>4</sup>	\$8,000	1	1	\$8,000
Oil change	\$150	1	1	\$150
Turbo pump felts	\$60	1	1	\$60
Filament	\$400	1	1	\$400
Sealing Gasket	\$100	1	1	\$100
<b>Total</b>				<b>\$8,710</b>

**Total cost, consumables and maintenance items \$24,097**

1. Assume 1 sample per vial, 6 injections per sample
2. Assume 20ml lasts for 1 year
3. 300 cu ft
4. Could be performed by experienced users-Instrument will be down for a week on average

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