## Mass Spectrometry & Spectroscopy

## Money To Burn: Do you Know What is Costs to Run your Atomic Spectroscopy instrumentation?

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You've been using flame atomic absorption (FAA) and/or electrothermal atomisation (ETA) for as long as you can remember. Very gradually, your trace element workload has been increasing and there is now a demand to get lower limits of detection. You think an inductively coupled plasma mass spectrometer (ICP-MS) will be the best option, but you've heard that it's much more expensive to run. What do you do? Purchase an ICP-MS and accept it will be more expensive to run, invest in an ICP optical emission system (ICP-OES) or just stick with what you know and buy more AA equipment. How often are lab managers put in this position, without really knowing what it costs to run these higher price-tag trace element techniques?

So to get a better understanding of these kinds of questions, let's take a closer look at what it costs to run each of the techniques. For the purpose of this evaluation, let us make the assumption that the major operating costs associated with running AS instrumentation are the gases, electricity, and consumable supplies. For comparison purposes, the exercise will be based on a typical laboratory running their instrument for 2½ days (20 h) per week and 50 weeks a year (1000 h per year).

These data are based on the cost of gases, electricity, and instrument consumables in the United States in 2016. They have been obtained from a number of publically-available commercial sources, including suppliers of industrial and high-purity gases, independent utilities companies, a number ICP-MS instrument vendors and sample introduction/ consumable suppliers). It's also important to emphasise that these costs might vary slightly based on the different vendor instrument design/technology/ being used.

#### Gases

FAA: Most flame AA systems use acetylene ( $C_2H_2$ ) as the combustion gas, and air or nitrous oxide ( $N_2O$ ) as the oxidant. Air is usually generated by an air compressor, but the  $C_2H_2$  and  $N_2O$  come in high-pressure cylinders. Normal atomic absorption grade  $C_2H_2$  cylinders contain 380 ft<sup>3</sup> (10,760 L) of gas.  $N_2O$  is purchased by weight and comes in cylinders containing 56 lb of gas, which is equivalent to 490 ft<sup>3</sup> (13,830 L). A cylinder of  $C_2H_2$  costs approximately \$200, whereas a cylinder of  $N_2O$  costs about \$70. These prices have remained fairly stable over the past few years. Normal  $C_2H_2$  gas flows in FAA are typically 2 L/min when air is the oxidant and 5 L/min when  $N_2O$  is the oxidant.  $N_2O$  gas flows are on the order of 10 L/min.

Air– $C_2H_2$  mixtures are used for the majority of elements, whereas an  $N_2O-C_2H_2$  mixture has traditionally been used for the more refractory elements. So, for this costing exercise, we will assume that half the work is done using air– $C_2H_2$ , and for the other half  $N_2O-C_2H_2$  is being used. Therefore, a typical laboratory running the instrument for 1000 h per year will consume 16 cylinders of  $C_2H_2$ , which is equivalent to \$3200 per year, and 22 cylinders of  $N_2O$  costing \$1500, making a total of \$4700.

ETA: The only gas that the electrothermal atomisation process uses on a routine basis is high-purity argon, which costs about \$100 for a 340 ft<sup>3</sup> (9630 L) cylinder. Typically, argon gas flows of up to 300 mL/min are required to keep an inert atmosphere in the graphite tube. At these flow rates, 540 h of use can be expected from one cylinder. Therefore, a typical laboratory running their instrument for 1000 h per year would consume almost two cylinders costing \$200.

Note: When liquid argon is stored in a Dewar vessel, there is a natural bleed-off to the atmosphere when the gas reaches a certain pressure. For this reason, a bank of argon cylinders is probably the best option for laboratories that do not use their instruments on a regular basis. Some of the newer ICP-OES instruments operate at approximately 60-70% argon consumption compared to older instruments. So this should be taken into consideration if this technology is being used.

Another added expense with ICP-MS is that if it is fitted with collision/reaction cell technology, the cost of the collision or reaction gas will have to be added to the running costs of the instrument. Fortunately, for most applications, the gas flow is usually less than 5 mL/min, but for the collision/reaction interface approach, typical gas flows are 100–150 mL/min. The most common collision/reaction gases used are hydrogen, helium, and ammonia. The cost of high-purity helium is on the order of \$400 for a 300 ft<sup>3</sup> (8500 L) cylinder, whereas that of a cylinder of hydrogen or ammonia is approximately \$250. One cylinder of either gas should be enough to last 1000 h at these kinds of flow rates. So, for this costing exercise, we will assume that the laboratory is running a collision/reaction cell/ interface instrument, with an additional expense of \$650.

It should also be pointed out that some collision/reaction cells require high-purity gases with extremely low impurity levels, because of the potential of the ¬contaminants in the gas to create additional by-product ions. This can be achieved either by purchasing laboratory-grade gases and cleaning them up with a gas purification system (getter), or by purchasing ultra-high-purity gases directly from the gas supplier. If the latter option is chosen, you should be aware that ultra-high-purity helium (99.9999%) is approximately twice the price of laboratory-grade helium (99.999%), whereas, ultra-high-purity hydrogen is approximately four times the cost of laboratory-grade hydrogen.

### Electricity

Calculations for power consumption are based on the average cost of electricity, which is currently about \$0.10 per kilowatt hour (kW/h) in the United States. The cost will vary depending on the location and demand, but it represents a good approximation for this exercise. So the following formula has been used for calculating the cost of electricity usage for each technique:

Cost per kW hour (\$) x Power Consumption (kW) x Annual Usage (h)

FAA: The power in a flame AA system is basically used for the hollow cathode lamps and the onboard microprocessor that controls functions like burner head position, lamp selection, photo multiplier tube voltage, grating position, etc. A typical instrument requires

ICP-OES and ICP-MS: The consumption of gases in ICP-OES and ICP-MS is very similar. They both use a total of approximately 15–20 L/min (~1000 L/h) of gaseous argon (inc. plasma, nebuliser, auxiliary and purge flows), which means a cylinder of argon (9630 L) would last only about 10 h. For this reason, most users install a Dewar vessel containing a liquid supply of argon. Liquid argon tanks come in a variety of different sizes, but a typical Dewar system used for ICP-OES/ICP-MS holds about 240 L of liquid gas, which is equivalent to 6300 ft<sup>3</sup> (178,000 L) of gaseous argon. (Note: The Dewar vessel can be bought outright, but are normally rented.) It costs about \$350 to fill a 240 L Dewar vessel with liquid argon. At a typical argon flow rate 17 L/min total gas flow, a full vessel would last for almost 175 h. Again, assuming a typical laboratory runs their instrument for 1000 h per year, this translates to 6 fills at approximately \$350 each, which is equivalent to about \$2100 per year. If cylinders were used, about 100 would be required, which would elevate the cost to almost \$10,000 per year.

less than 1kW of power. If it is used for 1000 h per year, it will be drawing less than 1000 kW total power, which is ~\$100 per year.

ETA: A graphite furnace system uses considerably more power than a flame AA system because a separate power unit is used to heat the graphite tube. In routine operation, there is a slow ramp heating of the tube for ~3 min until it reaches an atomisation temperature of about 2700°C, requiring a maximum power of ~3 kW. This heating cycle combined with the power requirements for the rest of the instrument costs ~\$300, for a system that is run 1000 h per year.

ICP-OES and ICP-MS: Both these techniques can be considered the same with regard to power requirements as the RF generators are of very similar design. Based on the voltage, magnitude of the electric current, and the number of lines used, the majority of modern instruments draw about 5 kW total power. This works out to be ~\$500 for an instrument that is run 1000 h per year.

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#### Consumables

Because of the fundamental differences between the four AS techniques, it is important to understand that there are considerable differences in the cost of consumables. In addition, the cost of the same component used in different techniques can vary significantly between different vendors and suppliers. So, the data has been taken from a number of different sources and averaged.

FAA: The major consumable supplies used in flame AA are the hollow cathode lamps. Depending on usage, you should plan to replace three of them every year, at a cost of \$300-500 for a good quality, single-element lamp. However, if a continuum source AA system is being used, there will not be a requirement to replace lamps on a regular basis. Other minor costs are nebuliser tubing and autosampler tubes. These are relatively inexpensive, but should be planned for. The total cost of lamps, nebuliser tubing, and a sufficient supply of autosampler tubes should not exceed \$1500–2000 per year, based on 1000 h of instrument usage.

ETA: As long as the sample type is not too corrosive, a graphite furnace AA tube should last about 300 heating cycles (firings). Based on a normal heating program of 3 min per replicate, this represents 20 firings per hour. If the laboratory is running the instrument 1000 h per year, it will carry out a total of 20,000 firings and use 70 graphite tubes in the process. There are many designs of graphite tubes, but for this exercise we will base the calculation on platform-based tubes that cost about \$50 each when bought in bulk. If we add the cost of graphite contact cylinders, hollow cathode lamps, and a sufficient supply of autosampler cups, the total cost of consumables for a graphite furnace will be approximately \$5000–6000 per year.

ICP-OES: The main consumable supplies in ICP-OES are in the plasma torch and in the sample introduction area. The major consumable is the torch itself, which consists of two concentric quartz tubes and a sample injector either made of quartz or some ceramic material. In addition, a quartz bonnet normally protects the torch from the RF coil. There are many different demountable torch designs available, but they all cost about \$600–700 for a complete system. Depending on sample workload and matrices being analysed, it is normal to go through a torch every 4-6 months. In addition to the torch, other parts that need to be replaced or at least need to have spares include the nebuliser, spray chamber, and sample capillary and pump tubing. When all these items are added together, the annual cost of consumables for ICP-OES is on the order of \$3000–3200.

ICP-MS: In addition to the plasma torch and sample introduction supplies, ICP-MS requires consumables that are situated inside the mass spectrometer. The first area is the interface region between the plasma and the mass spectrometer, which contains the sampler and skimmer cones. These are traditionally made of nickel, which is recommended for most matrices, or platinum for highly corrosive samples and organic matrices. A set of nickel cones costs \$700–1000, whereas a set of platinum cones costs about \$3000–4000. Two sets of nickel cones and perhaps one set of platinum cones would be required per year. The other major consumable in ICP-MS is the detector, which has a lifetime of approximately 1 year, and costs about \$1200–1800. When all these are added together with the torch, the sample introduction components, and the vacuum pump consumables, investing in ICP-MS supplies represents an annual cost of \$9,000-11,000.

The approximate annual cost of gases, power, and consumable supplies of the four AS techniques being operated for 1000 h/year, is shown in *Table 1*.

Table 1. Annual Operating Costs (\$US) for the Four AS Techniques for a Laboratory Running an Instrument 1000 h per Year (20 h per Week). (Note: 1 using a liquid argon supply, 2 using a collision/reaction cell)

| Technique | Gases (\$)           | Power (\$) | Consumable<br>Supplies (\$) | Total (\$) |
|-----------|----------------------|------------|-----------------------------|------------|
| FAA       | 4,700                | 100        | 1,750                       | 6,550      |
| ETA       | 200                  | 300        | 5,500                       | 6,000      |
| ICP-OES   | 2100 <sup>1</sup>    | 500        | 3,100                       | 5,700      |
| ICP-MS    | 2,750 <sup>1,2</sup> | 500        | 10,000                      | 13,250     |

#### Cost per Sample

We can take the data given in *Table 1* a step further and use these numbers to calculate the operating costs per individual sample, assuming that a laboratory is determining 10 analytes per sample. Let us now take a look at each technique to see how many samples can be analysed, assuming the instrument runs 1000 h per year.

FAA: A duplicate analysis for a single analyte in flame AA takes about 20s. This is equivalent to 180 analytes per hour or 180,000 analytes per year. For 10 analytes, this represents 18,000 samples per year. Based on an annual operating cost of \$6550, this

ICP-MS: ICP-MS also takes about 3 min to carry out a duplicate analysis for 10 analytes, which is equivalent to 20,000 samples per year. Based on an annual operating cost of \$13,250, this equates to \$0.66 per sample.

Operating costs for all four AS techniques for the determination of 10 analytes/sample are summarised in *Table 2*.

Table 2. Operating Costs for a Sample Requiring 10 Analytes, Based on the Instrument Being Used for 1000 h per Year (Note: 1 using a liquid argon supply, 2 using a collision/reaction cell)

| Technique              | Operating Cost for 10 Analytes per Sample (\$US) |
|------------------------|--|
| FAA                    | 0.36   |
| ETA                    | 6.50   |
| ICP-OES <sup>1</sup>   | 0.29   |
| ICP-MS <sup>1, 2</sup> | 0.66   |

It must also be emphasised that this comparison does not take into account the detection limit requirements, but is based on instrument-operating costs alone. These figures have been generated for a typical workload using what would be considered the average cost of gases, power, and consumables in the United States. Even though there will be geographical differences in the cost of these items in other parts of the world, the comparative costs should be very similar. Every laboratory's workload and analytical needs are unique, so this costing exercise should be treated with caution and only be used as a guideline for comparison purposes. However, it is a good exercise to show that there are running cost differences between the major AS techniques. If required, it can be taken a step further by also including the purchase price of the instrument, the cost of installing a clean room, the cost of sample preparation, and the salary of the operator. This would be a very useful exercise as it would give a good approximation of the overall cost of analysis, and therefore it could be used as a guideline for calculating what a laboratory might charge for running samples on a commercial basis.

#### **Final Thoughts**

It can be seen from this evaluation that based on the annual operating costs, FAA, ETA and ICP-OES are all very similar, with ICP-MS being approximately twice as expensive to operate. However, when the number of samples/analytes is taken into consideration the picture changes quite dramatically. It is also important to remember that there are many criteria to consider when selecting a trace element technique. Operating costs are just one of them, and they should not prevent you from choosing an instrument if your analytical requirements change, such as the need for lower detection limits. But, if more than one of these techniques fulfils your analytical demands, then knowledge of the operating costs should help you make the right decision.

#### Further Reading

1. R. Thomas, Practical Guide to ICP-MS: A Tutorial for Beginners, Third Edition, ISBN: 978-1-4665-5543-3 (CRC Press, Boca Raton, Florida, 2013). https://www.crcpress.com/Practical-Guide-to-ICP-MS-A-Tutorial-for-Beginners-Third-Edition/Thomas/9781466555433

#### Author Bio

Robert Thomas is principal of Scientific Solutions, a consulting company that serves the application and writing needs of the trace element user community. He has worked in the field of atomic and mass spectroscopy for more than 40 years and has written over 80 technical publications including a 15-part tutorial series and three textbooks on ICP-MS. He has an advanced degree in analytical chemistry from the University of Wales, UK, and is also a Fellow of the Royal Society of Chemistry (FRSC) and a Chartered Chemist (CChem). This article is an updated chapter from the author's book entitled 'Practical Guide to ICP-MS' published with kind permission from Taylor and Francis Group, a division of Informa [1].

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equates to \$0.36 per sample.

ETA: A single analyte by ETA takes about 5–6 min for a duplicate analysis, which is equivalent to approximately 10 analytes per hour or 10,000 analytes per year. For10 analytes/sample, this represents 1000 samples per year. Based on an annual operating cost of \$6000, this equates to \$6.00 per sample.

ICP-OES: A duplicate ICP-OES analysis for as many analytes as you require takes about 3 min. So for 10 analytes, this is equivalent to 20 samples per hour or 20,000 samples per year. Based on an annual operating cost of \$5700, this equates to \$0.30 per sample.





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