Traceability in testing labs.

(A metroloon dialogue)

Q: what's this traceability stuff, then?

A: what, isn't the VIM definition enough?

Q: that stuff about "related to defined standards" etc?

A: yes, that's the one.

Q: no, it's not enough! What "standards"? What's it for?

A: well, the first thing is what it's for. Look on it as one of the most effective ways of getting different people to get the same answer on the same sample.

Q: wouldn't they anyway?

A: only by accident. And most results are important enough that a difference can cost a LOT of money, or change a diagnosis or a court case. Or, of course, cause all your lab's customers to go somewhere else.

Q: Ah. So how do I make my results traceable, then?

A: that's easy. Make sure that every value that affects your test or calibration results comes from equipment or standards that are properly calibrated.

Q: Errmm...

A: look. You calculate your results from an equation. That equation always contains some values with units, like kg, m, mole, K. Those values all have to come from calibrated equipment, or from your certified reference standards. The only exception is values like instrument responses whose units cancel out - like a pair of peak areas that you ratio. I'll come back to those later.

Q: well, that's easy enough; get values in the equation calibrated. Thanks! 'bye!

A: Hey, wait up! I said Everything, remember?

Q: isn't the equation everything?

A: not usually. For most tests, the equation is only correct under special conditions, like at a particular temperature, or after a particular extraction or conditioning time.

Q: so? Doesn't the SOP have those things in?

A: exactly. And it specifies them because they affect the result. The result would be different if those things - I'll call them 'control parameters'- were mis-set.

Q: Aha. And if they affect the result....

A: That's right. They have to be from properly calibrated equipment too.

Q: And that's it?

A: well, if you've done all that, then yes, your results are indeed 'traceable'.

Q: hang on a bit. Loads of things must affect results. I'd be calibrating 'til doomsday if absolutely everything had to be calibrated. And what about all the stuff methods don't mention? I know weight is affected by atmospheric pressure, but none of my ordinary chemical test methods mention it at all.

A: true. But don't overdo it. Some of those things probably don't affect your answers much at all, compared to the accuracy you need, even if there's a theoretical effect. You don't really need to calibrate where calibration would make no practical difference.

Q: how do I tell?

A: well, one good way is to calculate the worst error that could reasonably happen. Use the natural range for a parameter like ambient pressure, and see how big the effect might be. Or you could assume manufacturing specifications (it pays to check them, of course).

Q: OK. So I only need calibrations for things that significantly affect my results, and some reasonable check on the borderline cases?

A: Yup. that's it.

Q: Great! So that's all I have to do to guarantee good measurements.

A: Oh dear. Not really. There are rather too many things that can go wrong if we rely on calibration alone.

Q: like what?

A: well, bitter experience shows that people actually do things differently even if they all follow the same SOP. And your kit could break. Or the test samples you're using could be quite different from the ones your method developer intended. Or if it's your own method, you need to make sure that the equation you're using is actually the right one. Or your instrument response might not be linear as you expect (I told you we'd get back to that peak area ratio- you usually need linearity for that to be useful).

Q: Oh wow. So what do I do about that lot?

A: well, you're probably doing it. Chemists call it validation. You do the best tests you can of your equation.

Q: "Best test"...?

A: Yes. A good test is independent of all the things you put into your equation. The ideal is to measure a sample with a value you know well.

Q: but if I've measured it with the same method, it's hardly independent, is it?

A: well spotted. No. Ideally, You need something someone else measured - preferably measured more accurately than you could.

Q: but why should I trust someone else's value to be the same as I'd get?

A: Excellent question! There's only one way: their measurement has to be 'traceable' too. that way, if you make things in your equation traceable, and they do too, the results SHOULD be the same (within your experimental uncertainties). If they are, good. If they aren't, one of you hasn't got a completely valid equation. Probably you.

Q: But one sample isn't much of a check...

A: no. Most people would want to do more. More independent traceable values (CRMs) if you can. If not, a comparison with another lab (even a PT scheme) is helpful. Or additional in-house tests; spiking studies, standard additions and so on. Ordinary method validation studies, in fact.

Q: Hmm. Does that mean my results are 'traceable' to all the things I've checked my method with? Do they make my results more 'traceable'?

A: Opinions vary on that point. In the strict sense of being part of the calculation of the individual result, clearly not. And it certainly is hard to work out whether, say, a comparison with another lab adds traceability to anything. In a less strict sense, maybe it does 'add' another traceability. But it doesn't matter much whether we call these checks 'extra traceability'. There is no doubt that each of these checks increases your confidence in the method and in your equation, and allows you to put more trust in the results you get with traceable equation values and control parameters. And that's the only real point of the independent checks.

Q: so that's it, finally? I get traceability if I've got calibrated values for everything I know can significantly affect my result, and I've checked that those things really are sufficient by doing the best independent tests I can?

A: Yes. Beautifully put.

Q: Good. So the only thing I need now is those 'reference standards'. What are they?

A: Various things. Pure certified reference materials or other certified analytical calibration standards are the main ones. The calibrated masses used for your balance calibrations cover mass. Temperature needs calibrated thermometers, and so on.

Q: But hang on a bit. Surely I only get 'traceability' to these things I buy?

A: no; that's the point of the calibrations and certificates. The values you get from these reference standards are themselves intended to be traceable to other, even more reliable references, and ultimately to the relevant global references. That way, ultimately, we all refer to the same reference points - and that's why traceability improves agreement.

Q: so it only works if it's all traceable, right to the top?

A: pretty much, yes. Some things are fairly easy to do well enough for routine use; a lot of simple organics, for example, can be shown (with care) to be better than 99% pure with good confidence without tracing further. And if we're sure enough that that is sufficient, we can stop there. But ultimately, traceability 'to the top' is the best way we currently know.

Q: Well, that seems to wrap up traceability pretty well. The only thing I don't see is why that traceability definition talks about uncertainty. Surely what we've been saying can be done without knowing anything about the uncertainty at each step.

A: You're right. The links are there, through calibrations, whether we know the uncertainty or not. So uncertainty is not fundamental to the idea of traceability. But that (the VIM definition) is a practical definition for working measurements, not a purely mathematical definition. And for real results to be useful, we need to know about their uncertainty. If you think about it, you can't really be more certain about your results than you are about the values that go into the calculation (and the control parameters). So to understand the uncertainty in our results - which we must do for correct interpretation - we need to know the uncertainty in the traceable values we use. And to get those, the people who certified them needed to know the uncertainty in _their_ reference standards, and so on. So to be practically useful, the uncertainties have to be known - all the way to the top. That's why it's in the VIM definition.

Q: OK. That even makes some sense. But there's only one uncertainty on my CRM certificate - it doesn't show all the separate steps.

A: No. The CRM supplier looks after the uncertainties in his standards, and includes them in his stated uncertainty, and so on up the chain. Just like you will when you calculate or quote uncertainties on your results.

Q: I will? How do I do that?

A: That's another story. But if you could refill this glass . ...