

Experiment & Sample Tracking Questionnaire

For Research Operations

Context

We are building a unified data platform for NETL that includes experiment and sample tracking capabilities. The goal is to digitize the workflow from sample preparation through irradiation, decay, counting, and analysis.

Nick Luciano has provided an initial list of sample metadata fields (shown below). We need your input to validate this list, understand current workflows, and identify any integration needs with scheduling systems.

Proposed Sample Metadata Fields (from Nick)

Nick suggested tracking the following for each sample:

- Sample Name (must be unique)
- Sample numeric ID (assigned automatically)
- Chemical Composition
- Isotopic Composition
- Density
- Mass
- Location of Irradiation (central thimble, lazy susan, etc.)
- Irradiation Facility (cadmium covered, etc.)
- Datetime of insertion
- Datetime of removal
- Decay time after removal
- Count Live time
- Total counts
- Total activity
- Activity by isotope
- Measurement raw data (spectra or other)

Commented [KS1]: What is the purpose of digitizing the workflow? Is this to benefit researchers doing similar experiments at NETL?

Commented [LN2R1]: Some benefit to researchers at NETL, but can also provide validation data to digital twin work.

Commented [SK3R1]:

Commented [KS4]: What do you mean by this? Do you mean solid/liquid/gas? Or something else?

Commented [LN5R4]: I mean the molecular formula. Like caffeine: C8H10N4O2

Commented [SK6R4]: This might not always be available - some of the work we do is unknown NAA samples. You might be better off just asking for a description of the sample - in terms of solid, liquid, gas.

Commented [KS7]: I would say this is the same thing - irradiation facility name should give you all the information. If you really want a separation, I would have irradiation facility be things like the central thimble, 3EL, etc. and irradiation location be either in-core or ex-core

Commented [LN8R7]: That's fine.

Commented [KS9]: I would rename these as follows:
1.Irradiation date
2.Irradiation time
3.Reactor power level

Commented [LN10R9]: I use datetime in the python sense. This is a data type that captures both the date and time.
Reactor power level is already being captured.

Commented [KS11]: This can likely be auto calculated by subtracting the irradiation date from the count date

Commented [LN12R11]: While we need a datetime for insertion and removal of the sample to match reactor behavior, we only need total seconds for decay time and count time. The decay time and the count live time are the total integrated time, like 3600s. So we can't subtract. Even so, I'd rather the user enter decay time explicitly, rather than infer it.

Commented [SK13R11]: Most users subtract the irradiation end date from the count start date to get that value using Excel. I'm not sure I understand what you mean by total integrated time.

Commented [KS14]: This is typically post-processing information and is usually kept by the researcher to analyze the data for whatever they're doing. It is not ...

Commented [KS15R14]: You'll also want to include the count datetime in addition to the livetime here if you are ...

Commented [LN16R14]: Regarding data kept by the experimenter and not recorded, we are hoping to offer ...

Commented [SK17R14]: If you're offering web calculators, you'll need to offer them for all the differen ...

Questions

Question 1

How are experiments and samples currently tracked?

Context: We want to understand the current workflow to ensure the new system improves rather than disrupts existing processes.

Follow-up: Is it spreadsheets, paper logs, a database, or ad-hoc? Can you share an example of current tracking (redacted if needed)?

Your Answer:

It's a combination of things. Some information – sample type (i.e., solid, liquid, gas), sample mass, maximum reactor power you might need (note this is not always what you irradiate at), irradiation time, facility, in-core/ex-core, etc. are recorded in reactor operations requests. However, depending on the irradiation you're doing, typically you include a variety of things you might do with that ops request so that it can follow cover more than one type of experiment. Especially for things like neutron activation analysis – that one covers a wide array of samples, sizes, etc. The ops requests also define expected doses from samples and any hazards (e.g., gamma emitter, beta emitter, fission product, etc.). Any fissioning samples we irradiate (e.g., uranium, plutonium, etc.) go through additional calculations to make sure we don't exceed our technical specifications limits for iodine and samarium. If you're using an ops request for multiple experiments, you're likely keeping track of the experiment details on your own – this can vary widely from person to person – spreadsheet, handwritten, etc.

During irradiations, each facility location has a binder that allows you to write in some information – date, time, researcher doing experiment, reactor power level, facility (if more than one is available at the location), dose rate – this is only used to record the dose rate of the sample when it is done being irradiated.

For post-processing data analysis, this is also researcher dependent and experiment dependent. Some things are done for customers, so we don't care about anything other than a rough estimate of what we produced before we ship it to them. In-house experiments for students or staff are typically analyzed in some way – that depends on the sample and what it emits. The way the data is analyzed depends on the researcher, but the most common is probably some type of spreadsheet.

Question 2

Are the metadata fields Nick listed above complete and accurate?

Context: Nick provided this list based on his understanding. We want to make sure nothing is missing and the field names match your terminology.

Follow-up: Are there fields to add? Remove? Rename? Are some fields optional vs. required?

Your Answer:

I left comments on the metadata fields directly for thoughts that I had. I don't see anything that needs to be added. Is there a reason you want the post-processing sample information as well?

Question 3

Should the system integrate with a scheduling/calendar system?

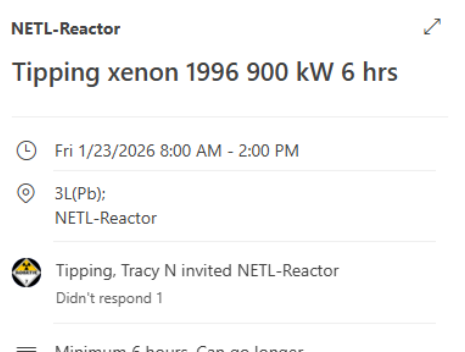
Context: Nick noted that a calendar shows intent (what was planned) while the tracking system should show what actually happened. However, linking them could be useful.

Follow-up: Do you currently use a shared calendar for scheduling reactor time? Would it be helpful to see scheduled vs. actual in one view?

Your Answer:

The way we schedule reactor time right now is send a calendar request to NETL-Reactor with our name, desired power level, estimated irradiation time, facility, and any details that might be important to the staff. They will then review that calendar invite and either accept or decline it.

Here's an example from this week:



I don't think it actually matters to any of us experimenters what the schedule says – we typically write down what happens on the day of for our own purposes and note down any changes that may have occurred. For example, when I was doing my PhD research, I used to request 8 hours of reactor time at 900 kW. But each time I did an experiment, I would note down the start time and the stop time – and also if I ever stopped early or did a shortened experiment.

Some requests – typically the pneumatic facility requests – are requested for longer periods of time, but actual irradiations are shorter or they do multiple irradiations in the timespan. For something like the TPNT/EPNT, you typically request a couple hours and then shoot multiple samples for a desired time (usually between 10 seconds and 10 minutes).

Question 4

What irradiation locations and facilities should be pre-populated?

Context: Nick suggested pre-populating dropdown menus for common options to speed data entry and ensure consistency.

Follow-up: Can you provide a complete list of: (a) irradiation locations (central thimble, lazy susan positions, etc.), and (b) facility configurations (cadmium covered, bare, etc.)?

Your Answer:

Ex-core:

1. Beam Port 1
2. Beam Port 2
3. Beam Port 3
4. Beam Port 4
5. Beam Port 5

In-core:

1. TPNT (thermal pneumatic facility)
2. EPNT (epithermal pneumatic facility)
3. RSR (rotary specimen rack) – this technically sits outside the reflector so it might be considered ex-core – but we usually call it in-core since it's inside the pool
4. CT (central thimble)
5. F3EL (fast 3-element facility)
6. 3EL(Cd) (Cd-lined 3-element facility)
7. 3EL(Pb) (Pb-lined 3-element facility)

I think that's all the facilities we have, but you'll probably want someone on the reactor staff to look this over. They'll know better than me. I've combined (a) and (b) in that list because that's how we always define these facilities – I don't think there's a need to separate them out. They're all unique facilities.

Question 5

What is the typical sample workflow from start to finish?

Context: Understanding the full lifecycle helps us design a system that supports each step.

Follow-up: Walk us through a typical sample: preparation → approval → insertion → irradiation → removal → decay → counting → analysis → disposal. What happens at each step?

Your Answer:

I would say this depends on the type of experiment happening and whether it's the first time we're doing something or if we've done it multiple times.

First time experiments have to do a complete safety analysis report and experiment authorization form before they can even do an ops request to run a sample. In some cases it also requires ROC approval if it is making major changes to the reactor. We have most recently done this for the cryo facility in BP2 and the F3EL. If you want more details on that I would recommend reaching out to Clayton Hudson – he did the cryo facility analysis.

If we're talking about a more general experiment, typically you'll go as follows:

1. Create an operations request
 - a. Run models (usually analytical or SCALE) to estimate the sample activities – go for conservative estimates (it's better for your sample to be slightly lower in activity than slightly higher). The modeling tells you what power levels/times you want to target for your irradiation to get a desired activity level.
 - b. Convert activities to dose rates – the reactor staff don't usually care about activity, they want to know how much beta and gamma dose they will receive handling these samples.
 - c. If you already have an operations request (noted with a 4-digit number – e.g., 1996 in the example I showed a couple questions ago), then you can reference that in your calendar request.
2. Create a calendar request – include name, power level, facility, 4-digit ops request, sample, irradiation time. The staff will review and approve.
3. On irradiation day – the staff will insert the appropriate facilities as needed or for ex-core experiments, you will set up your sample and let them know when you're ready. After they've completed start up checks, they will turn the reactor on, and you can begin your irradiation. During irradiation, experimenters will note down anything significant that may have occurred – they will also note down start time and stop time if they're doing longer irradiations. They also record the dose of the sample when it is finished being irradiated using a yellow frisker.
4. After irradiation, samples are pulled – when they are pulled depends on how hot they are and when they need to be analyzed/sent off. The medical isotope work we do is allowed to decay a little but pulled when still hot because it is a time sensitive project. This is something that is decided between the reactor staff and experimenter.
5. Analysis is heavily experimenter dependent – as part of our initial calculations we will determine when we need to count a sample and for how long. Some things can

be or need to be counted right away; other things have to decay first. Either way, you'll request the detector time you need or set up your own detectors for analysis. Anyways, most commonly, once you are ready to count your sample you will set it up on a detector and count it. You will do the respective energy and efficiency calibrations for your detectors as well.

6. Analysis is done in a variety of ways – whatever software you prefer for reading spectra. There's not a specific timeline for analysis – people do it whenever they need to – it doesn't have to be right away.
7. Disposal is done at the behest of the staff – usually when storage locations get too full. Again, this depends on the experiment – long-term experiments usually don't want to get rid of previously irradiated samples until the full project is complete. Some things can stay hot for a while and thus can't get disposed of for a while.

Additional Comments

Please add any other requirements, concerns, or suggestions for experiment tracking:

Thank you for your input! Please return this questionnaire to Ben.

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