
# *e*Science: Evaluating electronic laboratory notebooks in chemistry research

**Rosanne Quinnell and D. Brynn Hibbert**
Faculty of Science
University of New South Wales
**Andrew Milsted**
School of Chemistry
University of Southampton, UK

The School of Chemistry at UNSW is undertaking a trial of an electronic laboratory notebook (ELN) with selected honours and postgraduate research students. This ELN was developed at the University of Southampton and has been designed to accommodate the diversity of research in science. The concept of an ELN is that all the data from instruments, the observations of a researcher, their notes, thoughts, etc, will be captured within the ELN. The UNSW/Southampton ELN is a blog of each researcher's experiments, which resides on a secure server and is accessed through the web. It is intended that data will be readily retrievable for creating presentations, writing papers and ultimately the student's thesis. The project has obtained a number of input devices (e.g. netbook, tablet and notebook PCs, PDA) and will trial their use with the web site. The central part of this trial is the perceptions of staff and students as to the merits of adopting an ELN and the usefulness of an ELN to access experimental data more efficiently and to enhance communication between students and their supervisor(s).

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## Background

We predict that the 21st Century research chemist will be required to have a high degree of *e*Science proficiency, that is, to participate in online collaborative networks and to maintain productive research interactions with their colleagues through the exploitation of Web 2.0 technologies. Similarly, our research students will need to apply their IT skills to collaborative research as they begin their careers so that they can derive maximum benefits from the online domain. These predictions are based on the premise that open-access research blogs, digital object repositories and electronic 'mashups' seem to have hit the tipping point for uptake by the scientific research and teaching communities. We are rapidly leaving paper-based research behind us, with collaborative technologies, the online environment, and electronic laboratory notebooks replacing their non-electronic counterparts.

Some areas of science were 'early adopters' of collaborative technologies, and were first seen in the early 1990s (see Olson, Teasley, Bietz & Cogburn, 2002). From the late 1990s, research into global problems like climate change and epidemics such as HIV/Aids exploited collaborative technologies out of necessity. Olson, Teasley, Bietz and Cogburn (2002) explained that by the start of the 21st Century not all communities were ready for collaborative technologies and that for a successful collaboration there needed to be: a) collaboration readiness (where participants are willing to share information), b) collaboration infrastructure readiness, and c) collaboration technology readiness (including adequate technical support). Like any valuable discussion, a level of momentum within the collaboration, derived from the willingness of the participants, is needed for success.

In their research practice, scientists depend on sophisticated instrumentation for taking measurements. These measurements, which can number many thousands of data points, are tabulated and/or graphed by the instrument and saved as digital data files. Given that much of the instrumental data generated in science is in digital format, it would seem that operating in the electronic collaborative environment is a relatively easy step. But because: 1) legal requirements dictate that researchers log their experiments in a laboratory notebook; 2) the chemistry research community is diverse; and 3) we may not be providing our research students with sufficient infrastructure and opportunities to participate, it is unlikely that all areas of the community, or all participants, are ready to make the transition in full.

## Electronic laboratory notebooks

We are fortunate to have access to the ELN developed for research in chemistry from the University of Southampton. The Southampton Blog ELN was developed to be as flexible and simple as possible. Blogs were seen as a good analogy to the traditional laboratory book. The user is presented with a blank sheet, which is no different to a fresh page in their laboratory book. Unlike the ELNs that have been specifically designed for a single type of research e.g. myTea (Gibson, Stevens, Cooke & Brostoff, 2005), this ELN has been designed with sufficient flexibility to accommodate a range of experimental approaches and instruments, by adding tools such as cross-post linking, templates and attachment of data files generated by instruments such as mass spectrometers, spectrophotometers, fluorimeters and microscopes. A blog platform for the ELN has a bonus in that the ELN enables those who wish to partake in open science to publish their research at source (Neylon 2009, http://blogs.openwetware.org/ [accessed: November 9, 2009]). The Southampton ELN sandpit can be viewed at: http://blogs.chem.soton.ac.uk/bio_sandpit [accessed November 5, 2009].

The drivers to support implementation of ELN are:

- The ELN acts as a repository to archive digital and digitized experimental data with the data having a life beyond that of the researcher. This is important here because those who will be generating data are PhD students in chemistry, many of whom leave the institution after 3 – 4 years.
- All data and annotated experimental details are time and date stamped, and can be linked to related blog posts through metadata tags. Annotations are searchable for easy retrieval.
- Because the ELN is web-based it is straightforward for the institution to be responsible for the host server. A wider rollout of the ELN to allow shared access by different teams of researchers is simply a matter of creating accounts that can be accessed on the basis of the user's university credentials.

## Implementing the ELN technology

Given that this project speaks to implementation of a new technology that is situated in a 'learning and teaching' context, issues of pedagogy are required to be addressed. Radcliffe, Wilson, Powell and Tibbetts. (2008) offer a Pedagogy-Space-Technology framework to be used at an institutional level to enable "institutions to create new teaching and learning spaces that will encourage student engagement and improve learning outcomes." One aspect upon which the framework focuses is that the drivers for change (here referred to as 'motivation for the innovation') need to be articulated and that the initiative needs to be viewed through a scholarly lens. The team charged with implementing and initiating the trial is very much a trans-disciplinary group, which, according to schraefel, Hughes, Mills, Smith and Frey (2004), is the only way to bridge the gap in expertise of a design team and the domain expertise. We have expertise in how research in chemistry is undertaken; this is critical to set the priorities for implementation such as the required file format in which data is to be archived. We have expertise in the IT structure of the institution, which is required for the ELN to be compliant with institutional strictures.

Issues of physical distance have been implicated in the lack of uptake of initiatives such as this, with lack of distance being associated with poor uptake (Olson & Olson, 2000). So, if for this study, the students and staff are co-located, what makes us think that this initiative will be successful? First, we know that the discipline of science is very much based in collaboration (Biglan, 1973). Secondly, we are now ten years along from the study of Olson and Olson (2000); in those ten years have seen a considerable improvement and therefore uptake of technology upon which this project is based (e.g. Internet connectivity and now Web 2.0 environment) (see Caverly, 2001, for an interesting prediction of how technology would be used in the 21st Century in a higher education learning environment). Thirdly, we need to provide our students with authentic learning practices, which, for our research students, include exposure to 'collaboratories' that exploit Web 2.0 technologies for providing shared workspaces (Henri, Bédard, Hagemeister, Ghislain Lévesque, Kadri & Lessard, 2007). Web 2.0 technologies are considered to be key in realising authentic learning practices such as students contributing as knowledge-makers (Lombardi, 2007; Kreijns, Kirschnew & Jochems, 2003). Examining the process of interactions with shared workspaces is considered to be important to effective collaboration (Dourish & Belloti, 1992).

Aspects of the ELN technology that lend themselves to the practice of *e*Science in chemistry include:

- The ELN is a web application written in an open source blog language.
- Different input devices to be used within the laboratory to input blog entries into the ELN will be trialled and include notebook PCs, tablet PCs, web books, and two kinds of PDAs.
- The laboratories and offices in chemistry have been added to the university wireless network allowing access to the ELN from anywhere in the School.

We have identified elements that alert us to be cautious with the implementation. Our current concerns are:

- Security. There are perceived risks of keeping data on a server and the question of who maintains that server. Despite secure login there remains the question of who has really entered the data. Issues of fraud.
- Intellectual property and rights management. Do the procedures allow establishment of IP? How should the tension between users who support totally open access, and those who wish to keep their data private, be managed?
- Cost and resources. Set up includes costs of the server infrastructure, wireless coverage, and providing and configuring the devices to input data into the ELN. On-going costs include infrastructure upgrades, and IT management of accounts and training.

From a recent review of teaching and learning technologies at Bristol University (UK),

> …the ability to keep a well-ordered, neat hand-written record was an essential attribute for a practicing scientist, even if the environment in which they were working made use of electronic laboratory notebooks…(University of Bristol CELT Report 2007 p.41)

was put forward as the reason not to implement ELN at undergraduate level. This is not to say that information technology was not perceived as being important as the review went on to support the use of an online Dynamic Laboratory Manual (DML) by undergraduates. Importantly, the DLM retains the functionality of student access to their experimental data. What this report highlights is that we have not quite worked out how best to teach undergraduates the process of recording scientific information in a wholly digital environment.

## Project objectives

Our project will document the ELN implementation process the School of Chemistry at the University of New South Wales. We will identify how the alignment of the ELN system to the practice of research in science can be improved, i.e. what do students and staff consider to be the benefits and the limitations of e-environment to support their research in chemistry. We will use surveys to determine how 'technology-ready' the Australian academic chemistry community is to take full advantage of the collaborative technologies for teaching and learning. Is one branch of chemistry (e.g. organic, inorganic, analytical, physical) more 'technology-ready' than another to embrace 'born-digital' documentation for research? Or can any differences in willingness to adopt an electronic environment be explained by personal preference? Which collaborative technologies in particular (wiki, blogs, email, and repositories) are, or should, be incorporated into the student research experience in chemistry? Are our students more accepting of information and communication technologies in the research workplace than our academics? How well do collaborative technologies handle intellectual property and the legal aspects of research documentation? How well do students and staff manage their progress and the technologies when using e-notebooks for research student supervision as the student document research that culminates in a PhD thesis and peer-reviewed publications? Does an ELN enhance workflow in experimental research?

In July, 2009, we invited academic staff (n = 18) and postgraduate students (n ~ 56) in chemistry to complete an online survey to determine their willingness to use ELN and their perceptions of the usefulness and limitations of the ELN. In this survey we asked in which branch of chemistry they we researching. We used the first survey to invite students and staff to participate in a 12-month trial of the ELN (that commenced Sept 2009). At the end of the trial, we will invite those who participated to complete another survey, aligned to the initial survey. We will be able to a) compare the perceptions of those who did and did not want to participate in the trial and may be able to determine the most important sticking point for not adopting new technologies in a science research environment, and b) determine whether the perceptions of participants in the trial have changed, and if so, how. During the trial we have asked participants to blog (via the ELN) how they find interacting with the ELN blog. We will be able to ascertain the suitability of the different branches of chemistry for the adoption of ELN, the types of instruments and the file characteristics that are generated by these instruments (size and type). We will be able to compare the perceptions of students with the perceptions of staff in each branch of chemistry. Monitoring how students and supervisors participate in the process of sharing the virtual space, the ELN, we will be able to assess the effectiveness of student-supervisor collaboration within the ELN. Part of our work is to document the ELN implementation process at UNSW and to do this we are holding monthly focus groups.

## Initial feedback on this study

We have the results of the initial survey across the school although these are yet to be analysed in full. What we can report at this stage is that approximately 50% of students and staff have responded (27 out of 56 students; 10 out of 18 members of academic staff). The responses to the first survey have identified which instruments are critical to the students' research and we have used this information in discussions with those charged with managing the instruments in the school. The survey data are being used to inform the process of linking instruments such as NMR, UV-Vis and FTIR spectrophotometers to the ELN. At the level of the institution we now have expertise in the ELN, which is critical to ensure the people and the instruments can blog efficiently. Already we are sharing our implementation process in discussions with colleagues at other institutions.

In this study we have students and supervisors that are co-located, which, in the view of Olson and Olson (2000), is a powerful disincentive to use technology; if there is no 'need' then it is not used. However with research-active academics spending more time at conferences and being involved in more overseas collaborations, the ability to 'eavesdrop' on the progress of a student from anywhere in the world is a clear benefit of using an ELN. Other important drivers to the uptake are the improved access to instrumental datasets (e.g. after hours), coherence of data, the longevity of the datasets and their 'publication readiness'. We expect these drivers to over-ride the inertia due to co-location.

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**Authors:** Rosanne Quinnell, School of Biological Sciences, Faculty of Science, University of Sydney. *Currently* Faculty of Science UNSW. Email rquinnel@bio.usyd.edu.au

D. Brynn Hibbert, School of Chemistry Sciences, Faculty of Science, UNSW.
Email b.hibbert@unsw.edu.au

Andrew Milsted, School of Chemistry, University of Southampton, UK.
Email A.J.Milsted@soton.ac.uk

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