

Prague ELN days 2006

The search for an electronic laboratory notebook for research and teaching

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The Institute of Chemical Technology (ICT), Prague has long had a reputation for bringing their students into contact with concepts of scientific data handling which they will have to know and understand when they move into industry but which rarely find mention in run-of-the-mill curricula. Several years ago, they successfully deployed a commercial archiving solution to capture spectroscopic and other data from their analytical laboratories, which is in productive use amongst students and researchers.

In April they staged a two-day event which had the dual aims of educating key decision makers at the ICT and participants from other institutions in Prague as to various aspects of selecting an appropriate Electronic Laboratory Notebook (ELN). The Prague ELN Days was organised as part of the "Prague Centre for Innovations in Analytical Chemistry" Project financially supported by the European Social Fund and fiscal budget of the Czech Republic.

In an unusual and positive development, the vendors tendering for the contract were also allowed the opportunity to be present and interact during the presentations and to take part in the discussions around setting the priorities for the new solution. Their openness and expertise helped greatly towards making this event the success it was and I hope that the comments we received from the participants during both days will also help those vendors better understand the desires and aspirations

of their potential customers in the future.

Day One—background presentations

On the first day, two consultants, John Trigg, of phaseFour informatics and Chairman of the Royal Society of Chemistry–Automation and Analytical Management Group, and I, alternated presentations. In the morning, we covered a general introduction to ELNs before moving onto business issues, patent and intellectual property concerns in industry and academia including a series of case studies.

One of the hidden benefits that have been observed by those moving to this technology is the enhanced communication between chemists and analysts. If the ELN is deployed with appropriate access rights for the various departments, the Analysts are often in a position to do their jobs better as they can see deeper background information on the samples they are being asked to analyse. This in turn prompts the chemists to start to talk more to their supporting analytical staff about their own problems leading to a better, more productive working environment for both groups!

Pavel Matějka, the ELN project coordinator made it clear from the beginning that the ICT were looking to train students in systems similar to those they would find in industry and also manage the students' data from practical experiments as well as those from the research laboratories. The format

of the ELN Days was very open and after the morning sessions we asked the audience exactly what they were expecting from the deployment of an ELN in Prague. They responded that the ELN should:

- simplify work,
- help share information,
- standardise processes.

For the bachelor degree programme, the goals of the ELN were modest, with the intention of offering optional courses covering the flow of information in laboratory environments. The systems will be more intensively used by the Masters degree programmes with special laboratory exercises being offered around laboratory informatics and data management with special emphasis on the key features and benefits gained from using electronic laboratory notebooks. This will include advanced lab exercises. Finally, the PhD research students and their supervisors will move to electronic lab notebooks.

With the technology established, the ICT Prague will also serve as a centre of excellence in this new technology, offering seminars for academic staff and students from other Czech universities and members of the Czech Academy of Sciences. The close links that the ICT enjoys with industry will also be strengthened through this group starting to offer training courses and seminars for laboratory staff and decision makers from Czech chemical and pharmaceutical companies, as well as other chemical and analytical laboratories interested in

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learning the benefits of this new technology.

Cultural and technology issues

During the afternoon session, the seminar looked into the very important area of cultural issues surrounding the move from a paper-based lab notebook system to an electronic system. This change is one which needs to be managed very carefully as there are often unfounded fears amongst the users of such systems, so it is very important to emphasise the benefits that a user can achieve for their own jobs by making this change.

The afternoon continued with an overview of the improved position for long-term data preservation, which the deployment of an ELN brings. We looked into data migration strategies into the ELN, including the importance of the adoption of standards.

Implementation

Finally, we got down to the details of managing the implementation of an ELN—how the project should be best managed through various phases as well as how to assess and mediate the various risks involved. We looked at the reasons why similar technology projects fail such as:

- unclear objectives,
- scope creep,
- poor user acceptance,
- poor project management,
- technology doesn't work,

and discussed different tactics which should be adopted during the project from planning through design and development to the implementation to avoid making these mistakes.

Hopes and fears

The general discussion showed that, as should be expected from an organisation with a strong spectroscopic history, the need to handle analytical data was very much a high priority amongst the audience.

To wrap up we went around the room to discover what were the biggest hopes and fears amongst the participants and the responses were very revealing (see Table).

Biggest hopes	Biggest fears
Works for everyone and nobody complains	System starts and nobody uses it
New toy to play with—interesting opportunity	After 1 year it stops working and nobody knows why
Groups start to adopt it and we see measurable benefit	ELN suffers from differences between IT and the departments
I can improve my work, raise my profile amongst my colleagues	Other groups within the department don't accept the new system
The ELN improves information sharing with others	Deployment fails
The system allows us to share information better within the ICT but also with other countries	I won't be able to understand it
People find the system easy to adopt and useful	People don't adopt or the investment becomes quickly obsolete due to the speed the field is moving
I can increase my productivity by having better access to chemical property data	Some people spend too much time playing with the system and productivity drops
We will simplify our work and be able to get information on past experiments—say those done 10 years previously—we know those which were successful but it would be good to know those that failed so we don't repeat the mistakes	That we have enough money to buy the most appropriate product to suit the needs of all departments
The new ELN will work with no trouble—ever (user)	Data trusted to the system may become corrupted or destroyed—and that the system will be user unfriendly
All my work and results can become searchable from a single location	Human factors—not all data imported—data left on scraps of paper, hard drives
Simplify my manuscript writing (data not in different directories on various hard disks) all data and literature together cross-referenced but stored once	People who use/administer the ELN ask other uses to be made of the ELN platform
Get rid of piles of paper	System too sophisticated and therefore fails in our environment
Functionality allows it to be deployed within an educational environment and provide real experience for the Masters students	During startup the research can slow down—system failure after 2 years when the PhD students start to write up
Better research data sharing between students and supervisors	Confusion if the solution selected is too much of a hybrid or compromise between competing demands

Day Two—the vendors

On the second day the vendors showed off their systems with each allowed around 70 minutes to demonstrate their solutions and 10 minutes for a question and answer session with the audience. The excellent vendor presenters were Thomas Doerner (MDL Elsevier), Fredrik Rosengren (Contur), Stefan Seidler (Tripos), Christina Schroeder (CambridgeSoft) and Carsten Koblischke (Waters).

There was an interesting split of basic concepts which had been adopted by the various vendors when designing their ELN solutions. Some vendors have come into the ELN field from the chemical structure handling background and are very strong in this area. Others are building ELN solutions based more on their experiences in the laboratory workflow

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and laboratory information management sector where the need to handle chemical structures is given as much weight as the need to handle analytical data such as spectra or chromatograms.

The two days were regarded by all as a great success. In one respect, however, life was made more difficult for those trying to select which solution to purchase. This was highlighted by the comments by the audience on their feelings following the two days.

"I need two more days to get my head around all we have seen"

"My first time exposed to an ELN and I am surprised how much we can change in our work—I now have a lot of questions for myself, the vendors and the institute"

"Most useful for me, looking from the point of view of the common user I was surprised how many ways there were of doing things"

"We have seen many different approaches—designed for industrial companies and not academic environments—we have much work to do"

"2 days ago I knew nothing—I now have lots to think about"

"I've reviewed ELNs on the Internet but failed to find enough concrete information—this seminar has been essential to see what the different systems can really do—on the Internet it is not possible to see behind the marketing"

"This is my first experience of ELNs and in some areas they can do more than I expected but also in some areas less!"

All in all I think we all learned a lot from the openness of the discussion amongst the audience and the vendors for which all can be congratulated and I wish the ICT all the best in their difficult task of selecting a solution which will best meet their wide and varied demands!