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ABSTRACT

On the basis of long experience in teaching chemical literature courses, an integrated education and training program was introduced as a mandatory course in chemical information where both classical printed and modern electronic forms of information are covered. This mandatory course forms a standard part of the Institute of Chemical Technology (Prague, Czech Republic) chemistry curriculum. An important condition for designing this course was building a special classroom for teaching information technology. The classroom is located directly in the Central Library of chemical faculties, and includes computer access to local and distant information sources, sets of duplicate printed secondary reference sources such as Chemical Abstracts, Beilstein Gmelin, encyclopedias, and other materials available for teaching purposes. This paper describes the course objectives, technical prerequisites and requirements, database and software selection, language problems (since the majority of chemistry information is in English), provides the program syllabus, and describes initial experiences with this form of information education. The information program has been tested with more than 600 students who took the course mostly in their second year of study. The course was received favorably, and is now a standard part of the chemistry curriculum. (Author/SWC)

Integrated Information Education as Standard Part of University Curriculum in Chemistry

By:

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Integrated information education as standard part of university curriculum in chemistry

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Abstract: *On the basis of long experience in teaching chemical literature courses, an integrated education and training programme was introduced as an obligatory course in chemical information where both classical printed and modern electronic forms of information are covered. This obligatory course forms a standard part of the university chemistry curriculum. An important condition for designing this course was building a special classroom for teaching information technology which is located directly in the Central Library of chemical faculties, and where not only is computer access to local and distant information sources provided but also sets of duplicate printed secondary reference sources like Chemical Abstracts (complete five-year period with appropriate Collective Indexes), Beilstein Gmelin, encyclopaedias and others are available for teaching purposes. The syllabus of the programme is given and initial experience with this form of information education is presented.*

Keywords: Information education, printed and electronic technology, chemical information, syllabus, courses in information

1. Historical overview

Some kind of efficiency in extracting information from resources, handbooks, scientific periodicals and other materials has always been considered an important part of the overall professional prerequisite for scientific work in chemistry. A good knowledge of how to find important information has been valued perhaps more in chemistry than in any other scientific discipline, as can be well-documented by an extensive list of textbooks, monographs, manuals, instruction materials and other aids written on this subject (Ref 1).

But formal education in chemical information, or at least some kind of practice session for undergraduate or graduate students, has been conducted mostly individually, together with other subjects or as a part of laboratory exercises. Students have received the most intensive training in library usage when working in laboratories on a voluntary basis, or during preparation of their diplomas and theses. It was (and often still is) quite common and accepted for instructors and professors to take their students into the library to show them on the spot how to work with indexes and secondary reference resources, and where to find primary periodicals and factual data. A plethora of books on chemical information (or literature) is used mostly by research chemists when they realise that, being productive and efficient researchers, they need more detailed information on chemical information methods. This pattern was followed generally in our chemical faculties with the notable difference that we could not buy most of the manuals and monographs on chemical information published in Western countries. Therefore during this period a few such materials were published in the Czech language and, due to growing demand, in repeated editions (Ref 2). This situation with our chemical faculties is not essentially different to the situation in other countries. Zass stated that the number of chemistry departments offering formal instruction in chemical information retrieval is rather small in Germany (Ref 3).

It became slowly apparent that instead of leaving preparation for information retrieval to the individual it would be better to offer at least some form of formal course framework, e.g. a couple of lectures with subsequent practice sessions and preparation of a short review paper on a given subject to get a credit. Courses on Chemical Literature for which we had appropriate instruction materials had been taught this way for more than 20 years (Ref 4). A strong impact on formal education in this subject came after the indexing system in Chemical Abstracts was restructured and refined in the early 1970s. The separation of General Subject Headings and Chemical Substance Headings with a preselected hierarchical list of approved terms for volume indexes, and the open non-hierarchical terms used as keywords in Keyword Indexes, meant that some old practitioners were not able to locate information in Chemical Abstracts in the same manner as they used to be.

The advent of online technology in the former Czechoslovakia at the end of the 1970s, with a central intrastate database centre accessible by dial-up public telecommunication links, made possible the installation of early CA Online products such as CA Condensates and then CA Search (Ref 5). It was another incentive for the slow but steadily growing inclusion of information on online and other electronic services into the course on Chemical

Literature. Finally we decided it was time for a more radical rearrangement of the course on Chemical Literature into an integrated education and training programme, where both traditional printed and modern electronic forms of information would be presented in a comprehensive manner. Moreover, we suppose that it is also time for such a course to be included as obligatory in the standard university chemistry curriculum.

2. Main chemical information course objectives

We formulated three main objectives for the basic obligatory course on chemical information:

- the classical library with printed sources — books, encyclopaedias, periodicals, tables, handbooks and similar materials — will still be used in the foreseeable future and *students have to learn how libraries and their collections are organised, and how to use them*;
- electronic access to practically all kinds of information will grow rapidly, and *students have to learn how to use such access systematically*, not just accidentally by surfing the Internet or similar techniques. The main information sources for which usage has to be mastered in electronic form are the secondary reference databases such as Chemical Abstracts, Beilstein, Gmelin, Science Citation Index and others.
- for chemistry and many related disciplines *the computer representation of molecular structures is one of the key points of the whole system of chemical information*, and therefore it must be covered by the education and training programme.

In practice the first two objectives are closely interrelated: the third represents a somewhat separate and independent subject. We hope that by formulating these objectives for our course we set up priorities not only for the present situation but so that the hierarchy of objectives will survive developments in information technology for some time.

3. Technical prerequisites and requirements

It is clear that for any modern course on information retrieval and technology the possibility of practical work with computing facilities in a network environment is a fundamental prerequisite. For our programme we were able to build a lecture room designed specially for teaching and training of information technology. But what is perhaps more important is that the lecture room is located in our technical university's Central Library of chemical faculties: in other words, it is in a library environment. The natural interrelation between classical printed information sources and modern computer technologies may be displayed very clearly with plenty of practical consequences for training, demonstration and hands-on experience. The lecture room is equipped with computer/terminals for 10 or 20 students, with one computer with an LDC panel for the lecturer or instructor, all connected to the university network in a TCP/IP environment and through it to the Internet.

The interrelation of modern information technology with classical printed services and sources is further strengthened by providing this lecture room with spare sets of the most important printed information sources, like a full five-year set of the printed Chemical Abstracts volumes together with the set of Collective Indexes for the same period. This material comes from a cancelled subscription to CA in reorganised state information centres: we realised its enormous value for hands-on demonstration and usage training without disturbing the regular users of the printed Chemical Abstracts in the reading room of the Central Library. Besides Chemical Abstracts it was not too difficult to find duplicate volumes of other important printed sources — for example individual volumes of Beilstein's Handbuch, Gmelin's Handbuch, some encyclopaedias, older editions of some tables, and many other materials. Each student of the group can thus work with his or her own exemplar and all problems and tricks can be demonstrated on a real information source.

Summarising the technical requirements from the other point of view we can identify the following particular items:

- each terminal in the lecture room is an independent PC, with a set of standard software making it possible to train students not only to communicate with a database but to finalise results into the reports or tables, or to evaluate them statistically by means of other standard software;
- full connectivity to all local sources as well as to the Internet and database vendors, primarily to STN International;
- local Unix servers with loaded subscribed and licensed databases (e.g. CrossFire);
- a CD-ROM server on the local network providing access to databases or other materials on this medium (at present this uses the UltraNet CD/ROM networking technology based on copying the CD-ROM image onto a fast hard disk).

With this local and distant access technology available in the classroom, all possible methods of information retrieval may be taught, demonstrated and practised.

4. Database and software selection

When we are dealing with printed information sources there is practically no problem in selecting one particular product in preference over another. As in most chemical libraries in the world, the printed volumes of Chemical Abstracts with the appropriate indexes and the collection of primary journals represent the standard set of information resources used for both research and for teaching. The situation with electronic resources is much more complicated. Mainly for budgetary reasons it is not possible to have the full spectrum of important sources in both printed and electronic forms, or to buy most of the marketed databases or information system products even if they are very interesting and important. Beside the total price of a given product the most important factor for us is the possibility of using it without payment per use. In other words, we strongly prefer products which may be subscribed to and accessed as a local database on CD-ROM, or delivered on tape, or which may be accessed without limitation for a flat-fee subscription. Besides the self-evident reasons for such a policy, the still existing complication with cross-border payments of relatively small amounts, and the burden of often enormous bank charges, makes even cheap educational access policies such as the KR Dialog/Data-Star Classroom Instruction Programme (CIP) rather unattractive.

Being more specific, from this point of view probably the most important online information source for chemistry, STN International with CA databases, is difficult to teach effectively because STN does not have a flat-fee policy payment scheme. Therefore we can use only the STN Mentor product for online access demonstration and search simulation. On the other hand we are using the 12th Collective Index on CD-ROM extensively in our programme, and direct comparison of printed Collective Indexes with their electronic counterpart (even though it is not the same Collective Index) during classroom lessons is very helpful in understanding the indexing philosophy and rules. But we feel that the extensive database resources of Chemical Abstracts are not exploited for chemical information education and training as they should be.

The situation is quite the opposite with the factual databases from Beilstein and — though this does not yet apply in our case — Gmelin. The integrated package of both Beilstein's printed volumes with unlimited access to the electronic CrossFire version mounted on the local Unix server represents a very attractive solution for teaching not only information retrieval but organic chemistry itself. In our basic obligatory course on chemical information we teach CrossFire only on a very basic level, demonstrating predominantly the structure and substructure searches, but we found it to be an extremely motivating lesson for undergraduates. From this point of view the upgraded version, the CrossFire Reaction Plus which has the ability to search for reactions and to map starting material on products, would be still more attractive. As CrossFire has only been available for little more than a year on our local network the full potential is not yet exploited, and we expect its much wider involvement in different courses both on organic chemistry and chemical information methods. We expect the same development with the electronic version of the Gmelin database, which it has been announced will be mounted in the same CrossFire environment.

As we included not only the passive retrieval of information but also the active preparation or work-up of information in our programme, we have to select appropriate software products for such purposes. From the plentiful chemical text editors we rely on the standard MS Word 6.0, with ISISDraw for the preparation of structures or schemes for export into Word documents. In our programme we used the whole ISIS system for demonstrating reaction searches and for the design and development of structure databases, and we are negotiating with MDL for setting up some form of classroom access to the ISIS modules.

5. Language problems

For non-English speaking countries there is one problem sometimes overlooked concerning the language which is used for demonstrating information retrieval or the databases themselves. A not unimportant part of our programme is that early in the curriculum students are exposed to the fact that the vast majority of information, which is evidently indispensable in any chemistry-related professional work, is in English — or, to a lesser extent, in some other widely-used language. Our course is taught in the students' mother language, but for demonstration and when working with full or demo versions of databases or information systems, we pay no attention to the fact that the material is in English: we leave it to students to cope with this reality. This policy was adopted for a long time with hardly any complaints: on the other hand, the students often appreciate being confronted with the professional language reality early on.

6. Syllabus of integrated course in chemical information

The programme was designed for the present time allocation, which is two hours per week for one term (one semester, i.e. 14 weeks), which makes 28 hours altogether. This course is taken mostly in the second year of study, in the summer (fourth) semester. According to our lengthy experience this is the first suitable term. In earlier semesters students mostly do not realise the importance and impact of professional information, or they have only a superficial or one-sided knowledge of chemistry itself. There are four main blocks which correspond to the main objectives formulated above:

General subjects:

[1] introduction, basic concepts and elements of information processing and systems;

[2] the document as the most important form of scientific information;

[3] information technology, recording and storage systems;

[4] computer networks, local situation and global system, the Internet.

Chemical information, secondary reference sources, Chemical Abstracts:

[5] chemical information, history, specific features development and present status;

[6] basic secondary sources, the 'Handbuch' concept, Beilstein, Gmelin;

[7] abstracting and indexing services, Chemical Abstracts Service;

[8] primary document analysis, CA indexes system and their usage;

[9] comparison of printed and electronic indexes, online searching;

[10] system of CA databases, methodology and strategy of information retrieval;

[11] other databases, Science Citation Index, SDI and Current Contents approach;

Computer representation of structure, structure and reaction database:

[12] chemical nomenclature and computer representation of chemical structure;

[13] structure databases, exact and substructure search, reaction databases;

[14] 2D and 3D representation, ISIS system and database combination;

Additional subjects:

[15] patent information, basic facts about patents and patent systems;

[16] work-up of information data, evaluation, statistics and presentation.

It may be stated that at this moment roughly 50% of material is treated as printed sources and 50% as electronic sources, with a slow but steady shift to the electronic part. Credit is given on the basis of written tests with individual retrieval problems and a short review paper on a given simple subject. This form of programme has been in development for a couple of years: the final version presented has been tested with more than 600 students with quite favourable acceptance. At this moment there is no doubt about the integration of this course as obligatory for all chemistry students at our university.

7. Commentary on syllabus

It is necessary to add a few notes as commentary on the syllabus presented above. First of all we found the success of such a course depended on starting with very basic ideas, concepts and elements of information processing and information systems. Regardless of the fact that the modern world is flooded with information, students mostly do not realise how the information is formed, processed, stored, retrieved, disseminated, evaluated and finally used. It is very important to demonstrate clearly the cycle of scientific information, going from the known facts to new discoveries, and marking this route by correct citation praxis. Most students for the first time have the typical research paper in hand which should be their companion for their whole professional careers.

In the second block of subjects we concentrate on the main part of the system of scientific information, i.e. on the abstracting and indexing services and their products — the secondary reference sources regardless of whether they are used via printed volumes, or via online or CD-ROM media. Fortunately the Chemical Abstracts Service represents an ideal model for demonstrating and training in practically all the areas of such a business. From the other point of view, to teach students how to use Chemical Abstracts effectively in everyday work and in most practical situations without problems is without doubt one of the most important goals of this course. For this reason the time reserved for practising Chemical Abstracts in both printed and electronic form is greater than would follow from the syllabus. CA indexes are also very appropriate tools for introducing online search methodology and praxis, with the demonstration of basic steps from commands for login, through expand and search, to display. Unfortunately, due to the lack of some form of flat-fee payment scheme we can only use the Mentor module or a live demonstration by an instructor, without the possibility of students working online by themselves. It is rather a pity for we found that the instruction material for using CAS Database on STN covers the subject in an excellent manner and we are using it in many instances (Ref 6).

In this block there is also the common problem of going from citation in a secondary source to the location of primary information in its original form. Students are forced to decipher the full name of the primary source from its abbreviation, for which the CASSI Index is available and strongly recommended, and to find the original paper on the library shelves. Some mistakes introduced deliberately into the citation make an interesting exercise of the task, demonstrating the need to pay great attention to the correct citation.

The next most important subject is the computer representation of chemical compounds structure, starting from connectivity tables and going through drawing software and structure databases to the sophisticated reaction databases, in the last instance at the demonstration level only. Here the marketing strategy of the Beilstein Institute for its CrossFire product, based on a flat-fee budgeting policy, very substantially enhanced the possibility for practice sessions in structure manipulation. This part of the programme is both very attractive for the students and also helps in understanding some structure, reactions and in the case of the CrossFire database factual relations from general organic chemistry (e.g. to correlate structure with melting points or other properties of molecules). We suppose that still greater attention will be given to this part as some structure and reaction databases are now practically in the category of industry standard software.

As an additional subject we devote at least two hours to patent information, where the understanding of general problems is rather poor, and some time is also spent on the final work-up of data found using the standard software system.

8. Conclusion

While the idea of integrating classical printed and electronic forms of information into one formal course in chemical information has been developing slowly for some time, a more radical rearrangement of lectures and practice sessions could be realised after building the special classroom for teaching information technology inside the Central Library at our university. With such technical background and support available we had far greater possibilities for selecting course modules. Both students and instructors greatly appreciate the possibility to work, explain and discuss problems with authentic volumes and indexes of Chemical Abstracts in a classroom environment without disturbing other library visitors. Carrying such a course practically inside the library also offers many possibilities for demonstrating and training in many practical problems connected with real information retrieval tasks.

However, the practice sessions on computer and electronic information methods may also profit from immediate access to standard library resources, and can provide students with a good and reasonable feeling for the adequate selection and efficient usage of information resources and technologies. Summarising these favourable factors, we could introduce a formal course on chemical information as an obligatory course for all students in a basic three-year basic course of study in our chemical faculties. Until now the programme has been tested with more than 600 students who took this course mostly in the second year of study. The acceptance was quite favourable and the course is now a standard part of the university chemistry curriculum.

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