The Chemical Inventory System of the Center for Heterocyclic Compounds, University of Florida

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A system suitable for tracking the amounts and locations of ca. 10 000 chemicals is described.

INTRODUCTION

An inventory is essential for the correct tracking of supplies in any area, company, or organization. Since the beginning of the computer epoch, many such automatic general-purpose inventory systems have been created. The most recent have automatic inputs based on barcode technology. For a chemical inventory, it is possible to adapt a general-purpose inventory. However, specific features are required to track chemicals including (i) structure based search, in addition to searches based on nomenclature and trade name of compound, and (ii) substructure search, which is desirable especially for a research organization. In accordance with these requirements the chemical inventory system should be based on some chemical information database system which already has features of structure and substructure search. Until recently, there were no chemical inventory systems currently available with the provision of automatic input using barcodes. One available system CIS-Pro[1] based on ChemFinder[2] technology does not include barcode software and hardware interface.

We have developed our own inventory system (Chemical Index, CINDEX) based on MDL ISIS chemical information system.[3] Because of its scalability, reliability, and good ability to integrate with other softwares in comparison to other[2,4] chemical database management systems, we believe it should be of general interest. Our inventory system, which will be distributed free to noncommercial and educational organizations, provides much of functionality of recently available expensive, but universal systems (for example, SMART by MDL which began to be distributed after finalizing of our system).

THE ORGANIZATION OF CINDEX

The system includes two major parts: hardware and software. The hardware subsystem is based on a Percon PT 2000 barcode reader. The software subsystem consists of three parts: program for input processing; database; and barcode generator for new chemicals. The general view on the system is depicted in Figure 1.

Hardware and Software of Percon PT 2000 Barcode Reader. The nature of our chemical stockroom and chemical containers determined many of the requirements of our equipment selections. We chose the Percon PT 2000 with a PSC "Quickscan 6000 plus" and the optional "Autosense" stand. A hand scanner has the following advantages: it allows quick barcode scans, there is little dependence on technique, and importantly, there is no need for physical contact with contaminated bottles. Scanning wands are less expensive, but they are also less consistent and require close-to-contact scans which is inadvisable with bottles that may be contaminated.

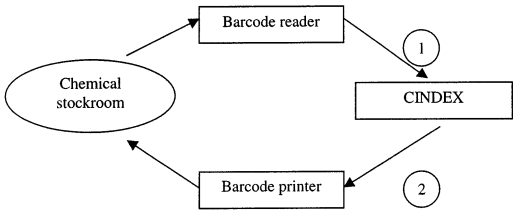

Figure 1. External dataflow in the CINDEX system.

We chose the PSC "Quickscan 6000 plus" because it meets the above criteria, it is economical, and has hands-free "Autosense" capability. Hands-free operation is essential for checking out chemicals in a laboratory environment, and the portability of a hand-held scanner is needed when performing stockroom or laboratory inventories. It is advisable to use a transparent cover to prevent the recorder from being damaged by exposure to solvents or other chemicals. An added bonus is that it uses standard AA NiCd batteries rather than expensive battery packs.

The PSC Percon 2000 portable data collector has an embedded programmable microprocessor. The program which we wrote for our inventory system was based on the "invpro.scr" program that was packaged with the PSC Percon 2000 along with several other demonstration programs. The algorithm of the program is depicted in Figure 3. The portable data collector is programmed so that the use of its various functions can be restricted to appropriate personal. This helps to ensure ease of use and that no one tampers with or accidentally deletes information. The program can work in three regimes: "chemist" (in which it is not possible to do anything else except scanning chemicals and chemists' CINDEX ID card) and two administrative regimes: "stockroom manager" (for additional scanning of the location during check in process) and "CINDEX manager" (with the possibility of transferring data to the PC and following deletion from device memory, full access).

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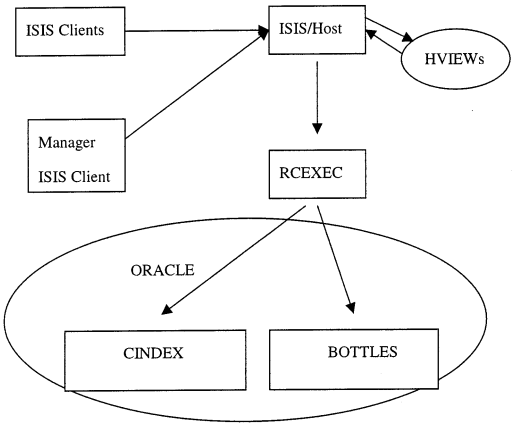

Figure 2. Organization of internal dataflow in the CINDEX system.

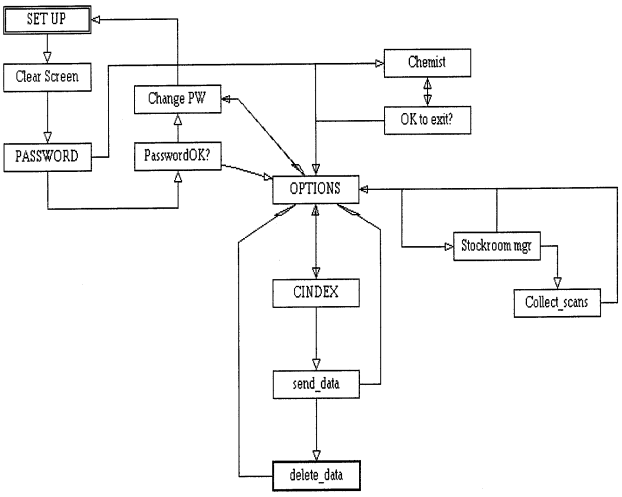

Figure 3. Barcode reader algorithm.

Input Data Processor. The processor is responsible for reading ROP files imported from PSC Percon 2000 device and automatically updates the CINDEX database. The program creates a registry (log) text file with description of all the performed actions. The program is realized on ISIS PL (Pascal clone) programming language. The algorithm of processing one line of ROP file can be described as follows: (i) find the corresponding subrecord in tree BOTTLES, (ii) update the location field, or (iii) (for check in only) update quantity if bottle is not empty or delete subrecord in opposite case. The operations are repeated for all lines until the end of file.

Database. The CINDEX database is ISIS/Host hierarchical database over ORACLE and consists of two trees: main CHEMICALDB tree with structural information and connected by value field CDBREGNO of the second-order tree BOTTLES with inventory information. Barcode data are saved in field BARCODE of the ORACLE table BOTTLES (the tree name BOTTLES, correspondingly)

Barcode Output System. The stickers (for our bottles and shelves) and chemist badges were created using the following:

(1) "MakeBarcodes" ISIS PL program which looks for empty field BARCODE in the subtree BOTTLES and then fills the fields using automatically generated unique code and prepares the list for the next stage.

(2) For this stage we use the specifically configured Barcode Anything software package.

The software package is not very versatile but is very intuitive. The 32-bit version is recommended because it can be used with Windows NT/2000 based systems. The software is compatible with Microsoft Excel, DBase, and many other common database programs.

ACTIONS

Searching of the Chemicals. For this operation we took advantage of MDL ISIS technology. The chemists search the chemicals using the ISIS/Base client from public computers in our group.

Check out. For check out, the chemist takes the bottle from the shelf and scans CINDEX ID. The bottle is then barcoded sequentially.

Check in. To return chemicals by chemists to the stockroom, we use a specially designated shelf. The stockroom manager sequentially scans the shelf code, level in the bottle, and the bottle barcode.

CONCLUSION

We have created a reliable automatic system for processing the inventory of the chemicals in our group. This system is allowed to support ISIS/Host server database in an up-to-date state with minimal human efforts. The average time of searching the chemical is significantly reduced; as a result the average productivity of our group has increased. This allows minimal waste of time on routine operations and gives more time for creative development.

REFERENCES AND NOTES

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(2) ChemFinder, CambrigeSoft Corporation.
(3) MDL ISIS Documentation package, MDL, 2000.
(4) U.S. Patent 5577239, Oxford Molecular, 1996.

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