T R O U B L E S H O O T I N G

LC User Survey: Data-System Problems

JOHN W. DOLAN

This is the final Troubleshooting discussion on responses to a recent *LC Magazine* reader survey (1). Previous columns reported the problems most commonly encountered with autosamplers (2) and detectors (3); this month, data-system problems will be addressed. For our purposes, *data systems* shall be defined as any device used to process data electronically from a liquid chromatographic run. The category includes inexpensive integrators that only plot chromatograms and report retention times and peak areas, as well as computer systems that collect and process data from multiple runs and control multiple liquid chromatography (LC) systems. Such a classification is justified because the wording of the questions and responses could not be correlated with specific data-system types.

LC data systems are perhaps the most frustrating piece of LC hardware because few chromatographers have the necessary skills to repair them, and, with the exception of those who have completed school within the last 10 years, few workers have any formal training in computer science. These frustrations are reflected in the results of the survey (Table I). Despite these problems, however, the experiences of other users, as reported in the survey, can provide insight into the purchase and operation of LC data systems.

EASE OF USE AND SOFTWARE PROBLEMS

Nearly one-third of the respondents indicated that they had problems operating their data systems, and several respondents specifically mentioned problems with the quality of the documentation supplied with their systems. Before purchasing a data system, study the manuals thoroughly to determine if you will be able to operate the system without assistance. *Menu-driven* systems generally are the easiest to use. They operate by a menu — a list of options presented on the display. The user selects an option and is prompted for information that must be entered before the system will function. Training by the manufacturer, preferably on your system in your lab, will help to overcome many of the problems that result from unclear manuals. Naturally, some systems are easier to use than others, but most data systems are not difficult to operate once you learn the command language required to solve your specific problems. If you don't use the system daily, it might be useful to write a step-by-step summary — in your own words — of how to operate the data system so that you don't have to hunt through a manual for instructions. It is important for you to be able to run the data system with confidence, or you will have difficulty separating operator error from system error when trying to isolate problems.

Many of the software problems reported in the survey were related to bugs and lack of flexibility. Most manufacturers try to debug software thoroughly during β testing in a "typical" customer lab before the software is released. The process is seldom complete, however, and most software undergoes one or two revisions during the first year of sales. You should weigh your need for a specific new software package against your willingness to put up with problems that have not been worked out by the manufacturer. When you do encounter a bug, carefully repeat the entry process to be sure that the problem is not the result of an operator error, then document the exact conditions leading up to the problem and report them in writing to the manufacturer.

Lack of flexibility in a data system is often a result of a poor buying decision. Before purchasing a data system, discuss with your colleagues the features you want in your system. Decide which of those features are essential and which are just "nice" to have. Armed with this information, you should be able to find a system that not only meets your present needs but also can grow to meet your future needs. The requirements of a quality-assurance lab that runs hundreds of similar samples each week are much different from those of a research and development lab that runs 20 different kinds of samples per week — one data system may not be able to meet the requirements of both labs. If you are contemplating the purchase of a recently released data system, be sure to see all of the important features demonstrated on a production model. (That will help you avoid buying mere promises of future improvements.)

In summary, try to identify software and ease-of-use problems before purchasing a data system. Ask the salesperson for a list of satisfied customers in your geographical area and get their impressions of the system. If possible, obtain some hands-on experience with a demonstration unit in your lab; if the system is "user-hostile" the first time you use it, perhaps you should try another model or brand. Remember, however, that even the best-designed data systems can be somewhat confusing until you become familiar with routine operation.

TABLE I: FREQUENTLY CITED DATA-SYSTEM PROBLEMS*

Problem Area	% of Total
Ease of use, software problems	32
Erroneous results	22
Downtime, service problems	22
Special features	14
Memory, data-loss problems	10

* some respondents cited more than one problem area (1)

ERRONEOUS RESULTS

Whereas the problems discussed above are made obvious by your inability to get the data system to operate, calculational errors can have hidden, yet disastrous, effects on the quality of the chromatographic data. Error in baseline selection when peaks are not fully resolved was a major complaint indicated in the survey. Two processes are important here: threshold selection and baseline determination. To determine whether a peak exists, the computer must be able to separate baseline noise from the start of a true peak. That is generally accomplished with a *threshold* or peak-sensitivity factor. The threshold value can be selected by the user in some systems, whereas, in others, it is selected automatically by the data system after running several minutes of blank baseline. If the threshold value is too low, the report will contain extra peaks that are actually noise. On the other hand, a threshold value that is too high will result in missing smaller peaks. It is better, of course, to have extra data than not enough, so errors in the threshold setting are best made on the low side.

The manner of drawing the baseline is subject to personal preference; therefore, data systems that don't select the baseline the same way you do can be frustrating. There are at least three ways to draw the baseline for a pair of peaks: drop a perpendicular line between the peaks to an extended horizontal baseline, connect the baseline before and after the peak

pair to the valley between the peaks, and "skim" the second peak from the tail of the first with a tangential baseline. Each method is valid under certain circumstances, and the best method to use often depends on your sample. Systems that restrict you to a specific method may give erroneous results.

Errors in the data system output can be reduced by testing the system with samples of known composition. Check the output for reproducibility and accuracy in retention-time reporting, peak identification, and area/height measurements. If the system's calculations are based on injections of standards, check those manually to be sure the results are correct. By thoroughly checking the system before injecting real samples, you can increase your confidence in the results. If errors are discovered in the internal calculations of the data system, contact the manufacturer for help.

DOWNTIME AND SERVICE PROBLEMS

Excessive downtime for LC data systems can be frustrating and expensive as work piles up or has to be repeated because of system failure. As with software problems, the amount of downtime for a data system generally is greater during its first year of availability than later when most of the bugs have been worked out. If system failure occurs, there are three general approaches to correcting the problem: on-site service by the manufacturer, depot repair at the manufacturer's facility, and repair by the customer. Vendors have different repair policies, and the decision to purchase a particular brand of data system should be based partially on information about servicing (4). On-site service is expensive, but it can be the most effective approach to problem solving if you can get a rapid response to a service request. The service engineer can witness the problem in your lab under your operating conditions — problems have a way of "disappearing" when you ship a system in for repair. The engineer can then either correct the problem or advise you on how to prevent it from happening again. Depot repair is effective and relatively inexpensive, but downtime can be extended if service turnaround is slow. Customer repair is often practical, even if the user has very little background in electronics, because most data systems are self-diagnostic, which helps isolate hardware problems quickly at the circuit-board level. A new board can be ordered by overnight courier; the user can plug it in, and the system will be operational the next day. When you are considering the purchase of a data system, be sure to check with other users about their experience with service support for that system.

SPECIAL FEATURES

The basic algorithms for peak selection, baseline determination, and area measurement have been used widely in LC labs for more than 10 years, so they tend to be the most reliable portions of data-system software. According to the survey, the added "bells and whistles" that contribute so much to the system's ability to interpret data can also be a source of frustration. Special software features that were reported as problem areas include graphics display, recalculation and replotting of peaks, summary reports from multiple runs, and accessing stored runs. Many users reported problems with multiple liquid chromatographs connected to a single data system or with set-ups in which several users rely on the same data system for results. On the other end of the spectrum was the user who had been oversold: "[the] system is larger than I need [and] therefore more confusing." Fortunately, most of the added data-system features can be ignored, and the system can function as a simple integrator for most systems.

MEMORY AND DATA LOSS

Unlike data recorded in a lab notebook, data recorded on magnetic media (for example, diskettes or tape) can be lost as a result of relatively minor accidents. A fingerprint or a little spilled coffee won't hurt your notebook, but it can destroy a week's worth of data on a diskette. Unless you have a battery backup for your data system, all the data that is stored in active memory (RAM) is lost when you turn the power off or if power failure occurs. For this reason, you should routinely (for example, after every sample) save important data, either as hard copy on paper or on a diskette (or hard disk). For long-term storage of data on diskettes, you should store the original and a copy in two different locations.

CONCLUSIONS

If there is a common thread that weaves through this discussion on data-system problems, it is that most of the problems are design oriented. With other LC components, most problems can be corrected through preventive maintenance and repair; data systems, however, are dependent on software, which cannot be "repaired" except by replacing it with updated versions. All of this points to the importance of selecting a data system suitable for your needs. Check with other users about system reliability, customer support, service, and ease of operation for the specific brand and model of data system that you are considering. Buy a system that meets your current needs but can be updated for future needs. Don't buy for the distant future, however; given the rapid changes in the computer field, it may be less expensive to buy a more powerful data system a year from now than to update your present system.

REFERENCES

(1) *LC Magazine User Survey VII* (Aster Publishing Corp., Springfield, Oregon, December 1985).

(2) J.W. Dolan, *LC•GC* **4,** 416–420 (1986).

(3) J.W. Dolan, *LC•GC* **4,** 526–529 (1986).

(4) J.W. Dolan and V.V. Berry, *LC, Liq. Chromatogr. HPLC Mag.* **2,** 508–513 (1984).

John W. Dolan is president of LC Resources Inc., of San Jose, California, and is a consulting editor for LC•GC.