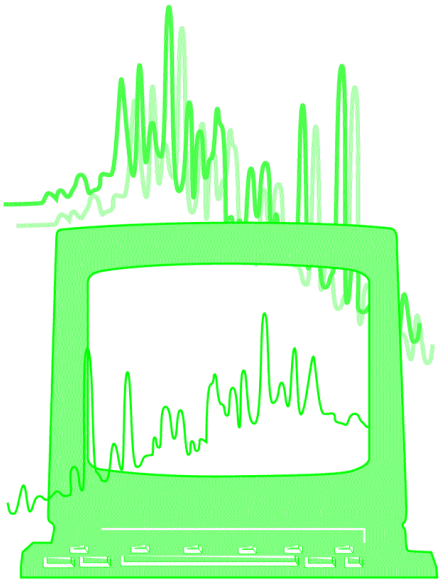
Chromatography Data Systems I: The Fundamentals



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Overview of the Series

Welcome to the first of a five-part series of articles about chromatography data systems (CDS). Chromatography data systems are used in many chromatography laboratories in many different industries.

We will look at a number of issues in this series:

- what is a CDS?
- specifying, evaluating and selecting a CDS
- validating a CDS
- maintaining the validated status of a CDS
- data migration and system retirement.

So why am I writing these articles? Chromatography data systems have been in laboratories for many years in many forms:

- integrator
- single PC
- central data system
- client/server or networked system.

Principles applicable to all types of data system will be discussed in this series. As they are generic rather than specific for a particular vendor or data system type, you will need to adapt some of the points to your specific situation.

Health Warning

Chromatography data systems are very useful in automating the quantification of analytes and are readily accepted as de facto within all laboratories that use chromatography. However, are things as good as they appear?

- How much do we know about the tools we use on a daily basis?
- How much do we take on trust just because a computer says these are the results?
- Do we really understand what a CDS does and the results it produces?

The purpose of these articles is to give an overview of what a CDS is and the functions it should perform. I'll also give you a bibliography of references for further reading.

Data generated from a computerized system and their limitations must be understood. There is an implicit belief that data generated by a CDS are trustworthy and reliable, especially if they are backed up with numbers expressed to six or more decimal places — nothing can be further from the truth!

Never believe that a CDS can save you from a separation with unresolved peaks. A data system must never be a substitute for poor chromatographic separation. Baselines and peak measurement algorithms use the same principles as manual quantification techniques. The only difference is that with a CDS these are automated and you believe they work!

Evolution of Chromatography Peak Measurement

A personal and selective view of how chromatographers have measured peaks over the decades is shown in Figure 1.

In the beginning…was the Jurassic Age of chromatography peak measurement: a chart recorder with a ruler and pencil. This is the baseline (sorry!) for measuring peaks — it is a slow, labour intensive and subjective process (e.g., placement of the baseline and the measurement of the height or peak width at half height is based upon the judgement of the chromatographer), but it is totally manual. One advantage of the pencil and ruler approach is that reasoning of baseline placement and measurement is recorded visually on the chromatogram itself providing an audit trail for others to follow the measurement rationale.

If this was too easy for the chromatographer, an alternative early method of peak measurement was cutting and weighing the actual peaks. The baseline was drawn on the peak outline, on the output from the chart recorder, and then the whole peak was cut from the chart recorder paper and weighed. This method relies on the accuracy of cutting out the peak, consistent paper density and humidity of the laboratory. However, if a supervisor does not believe that the baseline is correctly placed it is rather difficult to recalculate. Further information about manual peak measurement together with its advantages and disadvantages will be found in the book by Dyson (1).

The first attempts to automate peak measurement resulted in the production of the disk integrators linked to the chart recorders. Essentially these were electromechanical devices that linked the movement of the main pen of a chart recorder to a device that converted this movement into a second trace over on a calibrated track at the side of the main chart. Although this removes much of the tedium from peak measurement, a number of problems were found with this approach, such as the need for a stable baseline for accurate measurement (as the quantitative peak trace could drift otherwise). Furthermore there was usually a lag between the peak rise on the main chart recorder and the disk integrator response.

Microprocessor-based integrators were introduced in the early 1970s. Improvements in memory and the ability to measure peaks have expanded as microprocessors have developed. Integrators are dedicated devices for measuring chromatographic peaks and performing user-specified calculations, and also usually have a dedicated printer plotter to output the chromatogram. The program to run the integrator is located in firmware or Read Only Memory (ROM). The detector signal is fed into the integrator, parameters for data acquisition and processing are entered in, and away you go to coffee and leave the rest to the integrator. When you return, the integrator will have processed the signals from the injected samples and your results will have printed out. Memory problems with the early integrators meant that only the current chromatogram was stored, and if you wanted to replot it (change parameters etc.) you had to do that before the next injection wiped it out of memory.

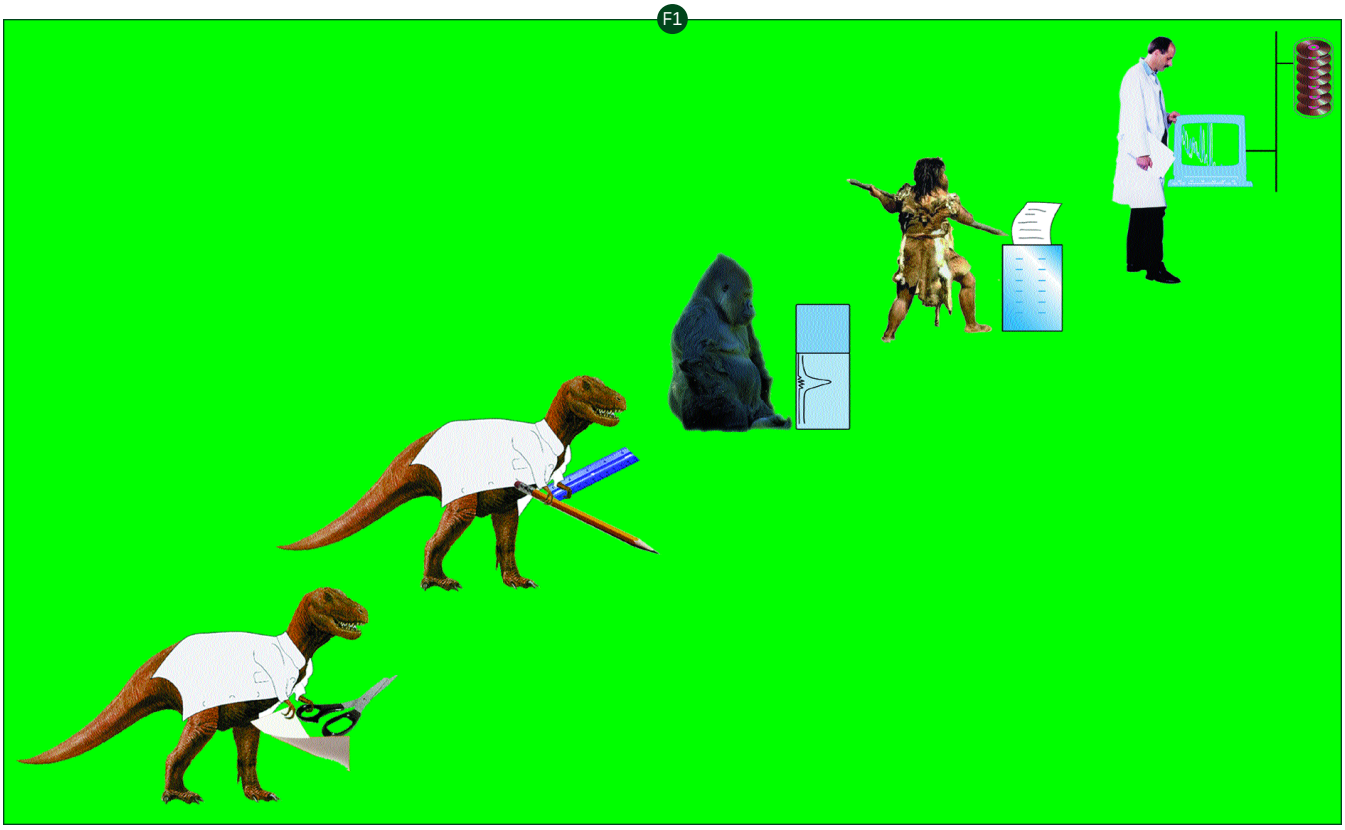

Figure 1: Evolution of peak measurement (after Darwin's theory of evolution).

Centralized data systems based on a host computer and multiplexed data processing were developed commercially by the mid 1970s for larger laboratories. Although relatively expensive, they allowed a laboratory to share methods and data files. Graphical reprocessing was possible, which had the advantage of reducing the need for sample reinjection. Following the development of client/server architectures, this type of CDS has been largely superceded by scalable PC network systems.

The arrival of the PC in the early 1980s led to the introduction of PC-based CDS within a year. The operation was similar to the integrator but data files from all injections of a run are now available for reprocessing with a PC and a centralized data system.

Advances in computing such as easy availability of high-performing PCs and networking have led to the availability of networked CDS. These and the single PC workstations tend to be the approach used today, and it is these types of data system that will be the main areas for discussion in this series.

What is a CDS?

A CDS has a number of functions that it can perform. These are dependent on the use of the system by the laboratory and the nature of the chromatographic equipment used (Figure 2).

In outline the process used by most CDS consists of all or most of the points below:

- Set up the method and analytical run information.
- Instrument control (dependent on the make of chromatographic equipment used by the laboratory).
- Acquire data from each injection, together with injection number from the autosampler and any chromatographic conditions.
- Process the acquired data first into peak areas or heights and then into analyte amounts or concentrations.
- Store the resultant data files and other information acquired during the run for reanalysis.
- Interface with other data or information systems for import of data relating to CDS set-up or export of data for further processing or collation of results.

We will discuss more detailed functions in each area later in this article.

However, there are a number of issues facing a chromatographer even at this level of detail:

- Should I have a number of stand-alone workstations or should I have a networked system? If I have a single

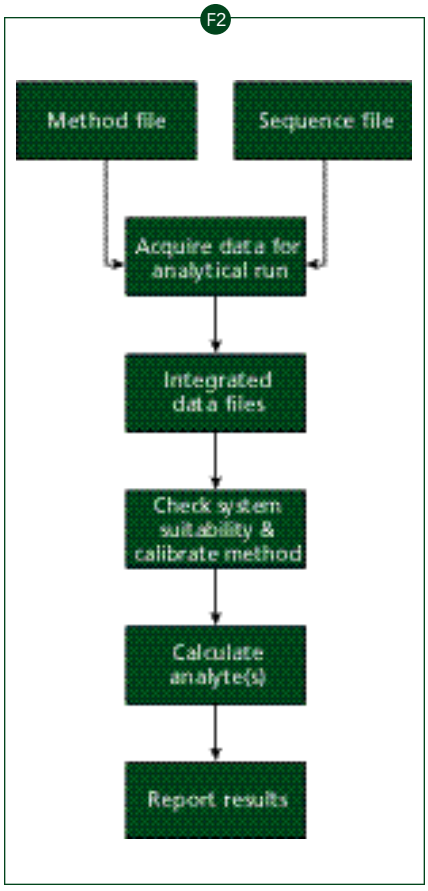

Figure 2: Functions of a CDS.

workstation how many instruments will I acquire data from and possibly control? Remember, if you have data acquisition from more than one chromatograph you will face keyboard contention: two or more people wanting to access the workstation to set up an instrument (usually in the afternoon/evening to set up a run) or to process results (usually in the morning). Ensure that the workstation is powerful enough to support both acquisition and reprocessing at the same time.

- How will I backup the data held on the system? Stand-alone workstations will need to be backed up individually on a regular basis, usually daily. A networked system, where data are held on a central server, will have this done automatically either via the system manager in the laboratory or by an IT department.
- Do I need to start naming conventions for my methods, sequence files and data files to help organize my results? As the number of methods and data files grows you are faced with two choices: to increase the number of disks to hold them all on-line or archive them to a suitable medium. If you need to retrieve a file and there is no naming convention, you may need to search.
- Furthermore, do I need to organize my data using directories via the operating system, or should I level this to a database working in the background? The traditional way to organize data files was to use directories and sub-directories; data acquired from a chromatograph would be collected and placed in a specific directory. However, either a user or the system manager needs to create the requisite directories and link the data channel to this. An alternative approach is to use a database to undertake the storage in a behind-the-scenes manner and a user just creates the folder in which their data will be stored. However, in my view, the use of databases in CDS has only just scratched the surface of possibilities and there are better things to come if only users want them.

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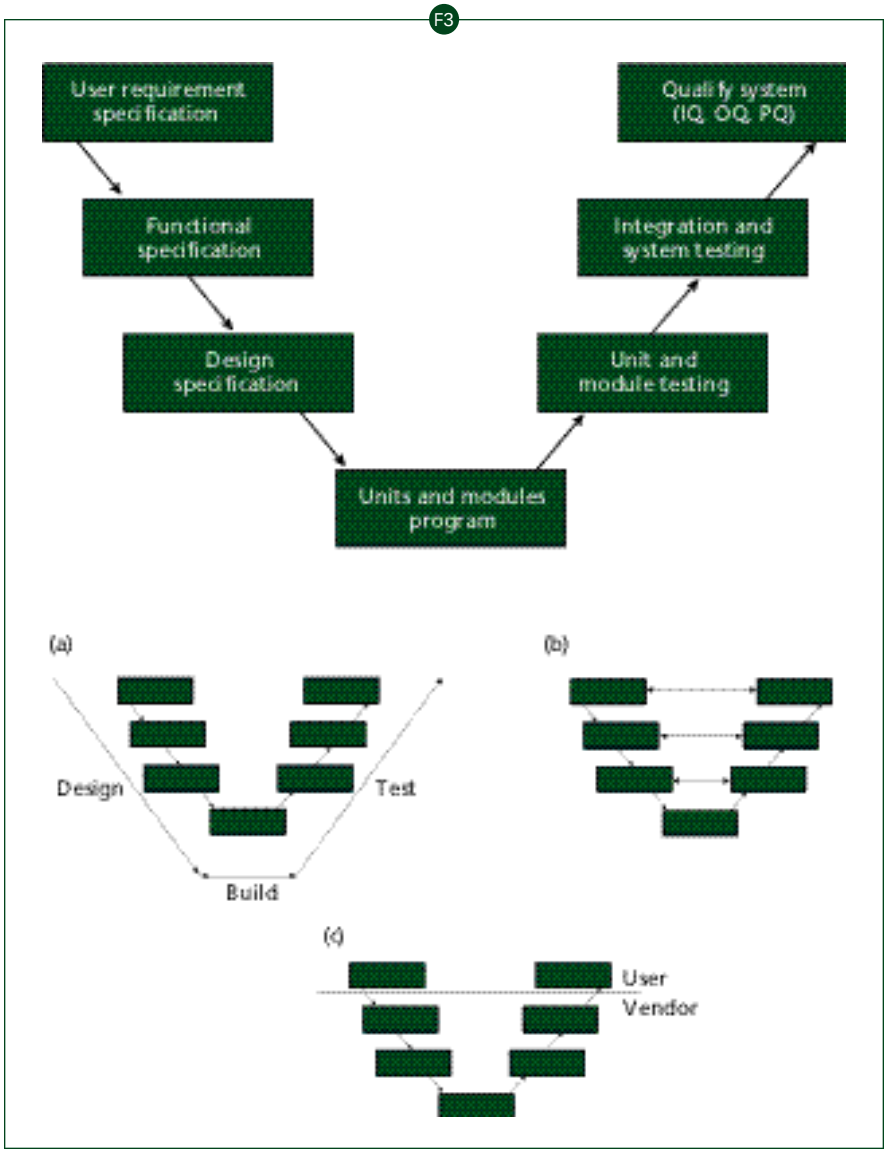

Figure 3: The ISO V model to describe a system development life cycle (SDLC).

Life Cycle of a CDS

This section is important and will be referred to throughout the series; please take the time to read it.

The life cycle that a CDS follows is no different to any other computer application. There are a number of models that can be used to show this:

- 4Qs model: design qualification, installation qualification, operational qualification and performance qualification. This, in my view, is adequate for equipment purchases, but it does not adequately describe the development of the software.
- Waterfall model described by the Institute of Electronic and Electrical Engineers (IEEE) is a cascade from a definition of requirements through development of software and release.
- The ISO 'V' model is my preferred model for any software application as it has a number of inherent advantages for describing the relationships between the various stages of software development. We'll spend a little time looking at this in more detail.

Features of the V model:

Design, build and test: The first is the very simple concept of design, build and test of the application (Figure 3(a)). The left-hand side of the V is concerned with design of the application; for our purposes, the CDS, but the model applies for any application. The bottom of the V is the system build: the programming of the units and modules, and the right-hand side covers the stages in the testing and user acceptance of the application.

Individual stages: Figure 3 shows the individual stages of the V model life cycle:

- User requirement specification (URS): specifies what the user wants the system to do. This is the basis of the user acceptance testing and qualification of the system.
- Functional design: this takes the user requirements and turns them into a computer programmer's view of the design for the system. This is an important stage that requires the crossing of disciplinary boundaries: chromatographer to computer programmer. From a vendor's perspective, the requirements of many laboratories are taken and incorporated into this document, so that they can produce a product with as much appeal to a wide range of potential customers.

- Design specification: further decomposition of the system design into individual units and modules of code. The function of each will be described, the inputs and outputs defined and the integration of all to produce the overall system.
- System build: the actual programming of the system. This should involve programming standards to ensure that the code can be easily maintained and updated in the future.
- Unit and module testing: As each unit and module is completed it should be tested, first by the programmer who wrote it and then by a second independent person. As units are integrated into modules, the modules will be tested and some of the unit tests reapplied to see if functions have changed (regression testing).
- System testing: When all modules have been assembled into a system there is usually a build version that is tested in-house (alpha testing). When the vendor is reasonably happy with the functions it will be released to selected users for beta testing and feedback. When all functions are working and it is relatively bug free the build is formally released as the next version and is available for distribution.
- Qualification: The new software is installed and the users test or qualify it to see if it is fit for purpose.

Time spent per stage: The model in its simplest form illustrates a flow down the left-hand side and up the right-hand side of the model. No feedback loops are shown in any of the figures illustrating the model in this article. However, do not be misled, because feedback loops exist. Their number and extent depend on the time the user or vendor has spent on the various stages. More time spent in the design stages means that the build and test will go more smoothly and quickly.

Rushing the design to meet a deadline may mean that items are incorrectly specified or missed out, and this may not be discovered until the test stages of the application development. Design or specification of a CDS is the inexpensive part of the life cycle for both the chromatographer and vendor. Missing or cutting short this stage means that either or both parties pick up the bill!

Relationships between stages: The V model is very useful for highlighting the relationships between the stages of the life cycle. Figure 3(b) shows these in outline: at the horizontal level the design phase is related to the corresponding test phase. For example, the design specification will outline the individual units and modules that will be coded and their functions. It will also outline how the individual units and modules will combine (inputs and outputs between them etc.) to form the whole system. Therefore, the unit and module tests that are applied will base their test design and acceptance criteria on the specifications in the design document. This relationship also applies to the other horizontal pairs in the model: functional specification and system test, and URS and qualification. This last pair is important from the perspective of the users as the URS defines the tests and their limits to be performed in the qualification or user acceptance testing. We will discuss this later in the series.

Moreover, the design stages on the left-hand side of the model represent a decomposition of the problem: requirements in the URS are broken down into functional requirements and then into design requirements for individual units and modules of a defined function. After programming, the test stages of the model on the right-hand side illustrate the building from these modules into a system ready for user acceptance testing.

User and supplier responsibilities: It is unlikely that you will be developing your own CDS; therefore, you will be purchasing a commercial system from a vendor. The V model is very useful in highlighting the responsibilities between the two parties. The users are responsible for the URS and the qualification or user acceptance tests, while the vendor is responsible for the remaining stages of the life cycle. This is illustrated in Figure 3(c) by the horizontal line. The user's responsibility is above the line and the vendor's is below. Again, we'll return to this area in later articles.

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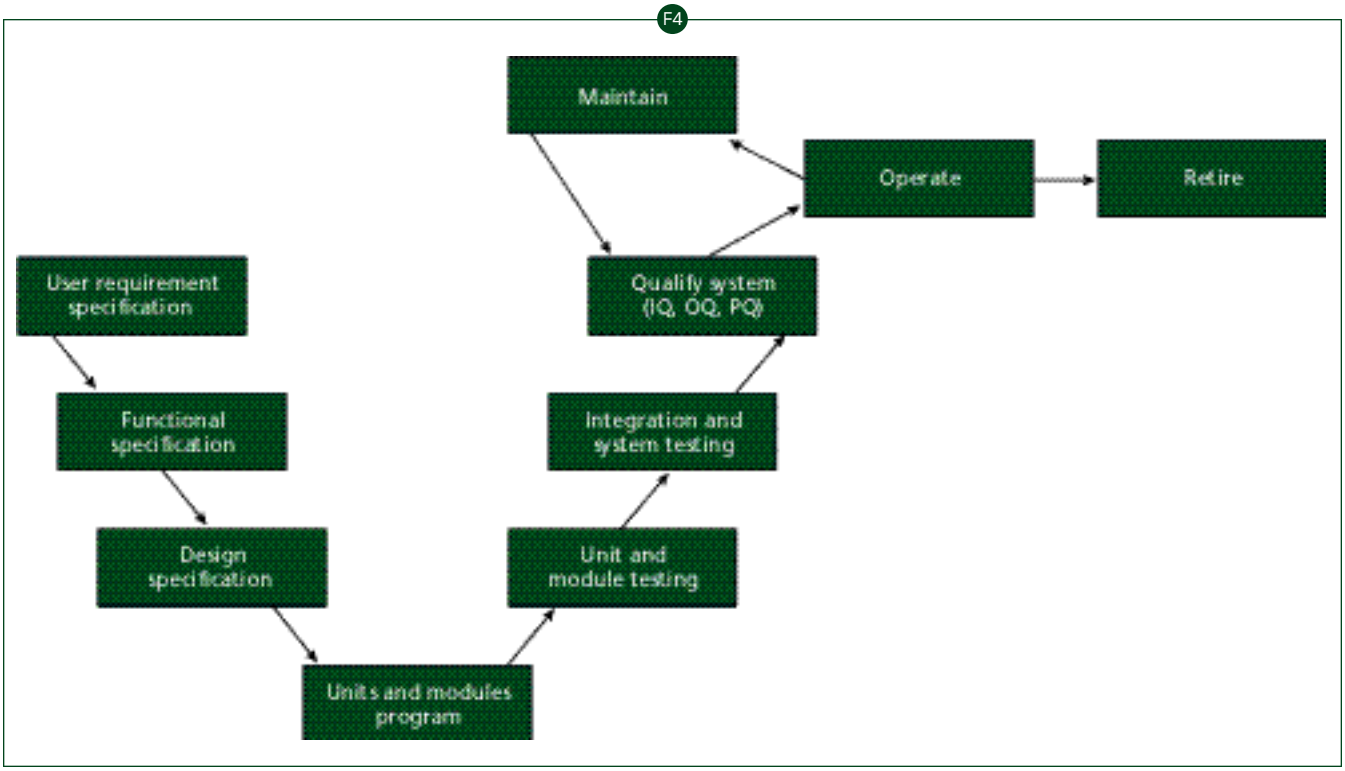

Figure 4: Modification of the ISO V model to incorporate operation and retirement of a system.

Limitations of the V model: While the V model looks good, there are some limitations to its use. As you can see, the model only covers the initial development of a system from the user specification until it becomes operational. For this it is very good, but this only represents a small fraction of the total time that a system is used. Some data systems can be operational for up to 20 years (including upgrades of the CDS software and the hardware platform); therefore, there should be a mechanism to accommodate this in the model.

The following life-cycle phases are missing from the V model:

- Operation: there are a number of tasks such as back-up, recovery, change control, configuration management, archive and restore that need to be covered in this part of the life cycle.
- Maintenance: every time an upgrade or change is considered to the system this part of the life cycle will be invoked.
- Retirement: when a system is finally retired and the data migrated to a new system or archived; there is no mechanism in the current model.

Therefore, to accommodate these later phases of the life cycle, the V model could be modified and look like Figure 4.

Functions of a CDS from Method Definition to Reporting

Referring to Figure 2, we'll work our way through the functions that a CDS could perform and highlight those that are not particularly well done. This is a generalized approach to the operation of a 'typical' data system: integrators have fewer functions available, and workstations and client/server systems will usually have more. As we go through this section think about how similar or not your laboratory is to this description:

- What is the routine operation of your laboratory?
- Are there any differences to the way you work?
- What differences do you need for method development: less formality and more flexibility?

The aim is to take this and adapt it to your particular operation and needs.

System set-up: Before an analysis can take place, both the CDS and any controlled equipment must be set up. This is achieved by defining the method for the analytical run in a method file, listing the samples to be injected in a sequence file and, where instruments are controlled, defining the appropriate experimental conditions.

Method file: The start of the data acquisition process is to build a method file that tells the CDS how to acquire data, process and interpret the results. A method file should include items such as:

- data acquisition sampling rate in the analogue-to-digital (A/D) converter
- when and how to integrate the chromatogram, such as if peak areas or heights should be used
- the baseline construction
- the identification of peaks
- the calibration method used to calculate analyte amount or concentration.

Ideally, if the method has been appropriately developed and validated, the method file should define the conditions so that the majority of the samples can be acquired and processed without the intervention of a chromatographer except to approve the results; that is, baselines are fitted automatically to save time manually reprocessing. Note the use of the word ideally. If you are to get the best from a CDS, the method must be well defined. Typical items to consider are baseline separation of all the main analytes and impact of the sample matrix (such as late-eluting peaks to avoid interference to subsequent samples).

Each method file should be uniquely identified, and whenever possible the version used for a specific analysis or sequence of samples should be readily achievable. Ideally, an authorized user should have the authority to create or modify a method. If a method has been modified then copies of the modifications must be stored with the data processed by that method.

Sequence file: The sequence file is the run list or order that the samples, standards, quality control samples and blanks will be injected into the chromatograph. Each sequence file or each injection must be linked with a method file to process the resulting data. For laboratories with large numbers of samples for a single method, the sequence file will usually be linked with a single method. Smaller laboratories or those requiring flexibility may link a sequence file with several methods during the course of a single analytical run.

A sequence or run file of the system is constructed initially using a series of create, copy and edit functions to input information such as:

- sample number
- sample identity
- laboratory number
- sample volume and internal standard amount
- number of replicate injections for each sample
- sample weights or volumes and any linked calculations for results.

Instrument control: Most chromatographers do not consider controlling their instruments with the data system. The larger data systems are capable of total control of a chromatograph. Originally this was provided that one vendor supplied both the CDS and the chromatographic equipment. However, as a result of user requests and pressure, the more popular types of instruments should be controllable from other vendors' data systems either now or in the near future. Alternatively, you may need special hardware, software or connections to achieve the same result.

Instrument control may vary from laboratory to laboratory and you may require all, some or none of the list below.

- Contact closures for the control of chromatographic valves or associated equipment during analysis are essential.
- Communication with the autosampler via binary coded decimal (BCD) or equivalent for sample continuity is in my view essential but is usually ignored by many.
- Remote set-up and operation of A/D devices.
- Remote set-up, operation and changing of operating parameters such as flow-rate, mobile-phase composition, detector wavelength etc.
- Remote monitoring of the chromatographic output that may include the instrument conditions.

Data acquisition: Analogue-to-digital conversion: The key part of any CDS is the process by which data are captured from the chromatographic detector for further processing. As this part of a CDS was the subject of a "Questions of Quality" column in December 1997 (5), it will not be discussed in any detail here. However, the key items to remember are

- The types of A/D unit commonly used in CDS are voltage-to-frequency conversion chips.
- Sampling rates, measured in Hertz (Hz) range from 1 Hz for conventional liquid chromatography (LC) to 5–20 Hz for capillary gas chromatography (GC), with possibly higher rates for capillary zone electrophoresis (CZE) depending on the peak widths involved. Normally a vendor will engineer a consistent high data capture rate (say 100 Hz) and then bunch the data when a lower rate is specified by the method. The data capture rate (also known as peak width) is one of the most important parameters for efficient integration of peaks.
  You'll need about 20 points to define a peak adequately. Too few will result in the peak being poorly defined and an error made in quantifying the peak.

Too many will result in difficulties determining the peak start and peak end, again resulting in error.
- Resolution is the smallest change in the analogue signal that can be seen in the digital output. The minimum resolution of a system should be 20 bits for conventional LC, but remember that if you have faster elution, a higher resolution may be indicated.
- Dual-channel data acquisition, as some of your methods may require the simultaneous use of two detectors per chromatograph; for example, ultraviolet (UV) and fluorescence. In these instances, is one channel slaved to another for purposes of data capture and can both channels of data be displayed on the same screen?
- Input voltages of the A/D unit should match the output voltages from the detector. When a large peak elutes there should be a message on the chromatogram that the input voltage was exceeded.

Data files, integration and processing:

Data files: The CDS must be able to store the data files and other information acquired during the run for integration, processing and, where necessary, reanalysis. A data file containing the sample slices will be obtained after each chromatographic run. It is important from scientific and regulatory considerations that digital files must not be capable of alteration. Moreover, they must not be overwritten either if the same sample information is assigned to an assay or if the disk becomes full.

Peak detection: The key stages in identifying a peak are shown in Figure 5. These are monitoring baselines to detect the possibility and recognition of a peak, the peak apex

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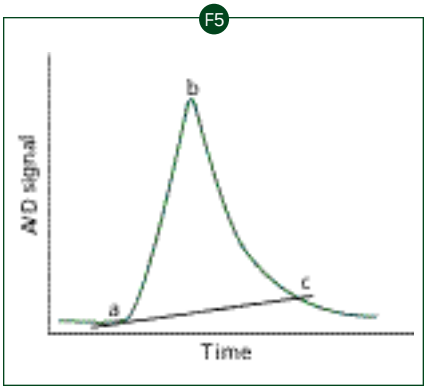

Figure 5: Peak detection. (a) peak is detected when increase in signal exceeds slope sensitivity; (b) apex defined, requires sufficient sampling points for accurate measurement; (c) peak end: detected when signal is less than slope sensitivity. However with tailing peaks baseline placement is often poor as in this example.

determination and the rear inflexion when the peak has eluted and the baseline becomes stable again.

Some of the issues that we need to discuss about peak detection are
- how a peak is detected
- minimum and maximum number of points required for peak detection and definition
- how data points are bunched to reduce noise or to help define slow-eluting peaks towards the end of a run.

The individual data slices in a file are analysed by the integration software using the parameters defined in the method file. Within the method file, some timed events will determine when the method will start to measure the peaks (integrate inhibit). This allows sections of the chromatogram to be omitted, such as the solvent front, and allows the chromatographer to concentrate on the peaks of interest.

Let us consider what happens to a single peak of interest and how a typical CDS will define the peak by determining the peak start, the apex and the peak end. This is the ideal situation.
- Peak start: The CDS algorithm will look for the rise of the detector signal rises above baseline, assuming that the data capture rate has been correctly set (see above). The sampling rate should be set to ensure 15–20 data points to define the peak adequately. A peak is detected when the rate of detector signal or slope increase rises above the minimum values set in the method file for the threshold parameter. If the threshold value is set too low, then noise can be detected as peaks; this is especially noticeable when you have a noisy detector signal. Equally so, if you set the threshold value too high then you will not detect small peaks of interest. Hence the need to develop and validate the method to the degree that is adequate for its application.
- Peak apex: The data capture rate must be correctly set for determining the apex of any peak. This is to ensure that the apex is correctly defined when the detector signal is rapidly changing. To ensure this, the data capture rate defined must be appropriate to the type of chromatography being undertaken (e.g., LC, capillary GC or CZE).
- Peak end: What goes up, comes down — eventually. Virtually all peaks in LC and GC are asymmetrical, the degree of peak tailing will depend on the interactions between the analyte and the mobile and stationary phases. The peak end is where the detector slope is zero within the limits defined by the slope sensitivity of the method. Where there is little noise and the data capture rate is suitable, there is little problem. However, where there is noise in the system or the data capture rate is too high, the placement of the peak end will be incorrect.

Peak integration: This is the process in which peak heights or areas are calculated from the defined peaks. The CDS will place a straight line between peak start and peak end to define the baseline. The signal representing the baseline at every data slice is subtracted from the total microvolt signal and the remaining values represent the peak. Peak height is simply the highest residual value in microvolts, which is printed out in the report at the end of the run. Peak area is the integration of the residual signals over the defined peak. The algorithms used for this will vary from vendor to vendor, are commercially sensitive and inevitably different, and can produce different results for the same input signals (3). The peak area units will be microvolts per second.

For the most accurate work, peak areas are preferred to peak-height measurements.

Once peaks areas or heights have been obtained, a calibration function is used to calculate the analyte amounts or concentrations. We will cover calibration in a separate section.

For more detail on CDS and how they detect and integrate peaks, I recommend the book by Dyson (1), which should be on the bookshelf of every chromatographer who uses a CDS.

Problems, Problems…There are a number of problems inherent with CDS that all users need to be aware of so that they can understand and overcome them.

Signal drift: Positive drift (the upwards drift of the detector signal) can be managed relatively well by most A/D converters. However, negative drift is a different situation. Most data systems measure the input voltage from a baseline of –50 or –10 mV. This will cope with some negative drift. However, bad instances of negative drift can exceed this. You should find out to what extent negative drift is accommodated by the A/D unit. Does this have any influence on peak detection? For example, if threshold value is used to detect peaks then this may be compromised with adverse negative drift. This means that drift can be detected as peaks.

The use of the autozero and offset functions can be used to minimize negative drift in an operational situation. You should look for a fall that turns into a flat baseline that indicates the signal has gone below the A/D lower limit.

Measurement of unresolved peaks: Here we have a major problem as most data systems only have two approaches to the measurement of fused peaks. These are either perpendicular drop or tangent skim (baselines here usually involve straight lines) (Figure 6). This approach dates back to the Jurassic Age of chromatography and is simply an electronic automation of the existing manual practice. Space does not permit a detailed discussion of the problems but inaccuracies and under-and-over measurement of peak areas are possible depending on the size ratio of peaks being measured. The reader is referred to the papers by Dyson (1, 2), Papas (3) and Meyer (4).

Calibration: Calibration is a weak area with most data systems. This is because chromatographers use many ways to work out their results. Often these methods are basic and lack statistical rigour, as the understanding of many chromatographers, where calibration is concerned, is poor. For instance a number of data systems have several calibration functions such as cubic, quadratic and log–log fits. In my opinion, there is no justification for using these models with conventional chromatography (e.g., LC with UV detection).

We will discuss this in more detail in part II of this series.

Presentation and reporting: Plotting and printing of chromatograms: Your data system should be capable of simultaneous on-screen plotting of at least two channels. Plotting should apply to both real-time as well as reprocessed data. The plot size should be variable with autoscaling, monitoring selected peak or user selectable ranges.

The plotting options of a basic data system should include

- fitted baselines
- peak start/stop ticks
- named components
- retention times
- timed events (e.g., integration start or inhibit)
- baseline subtract.

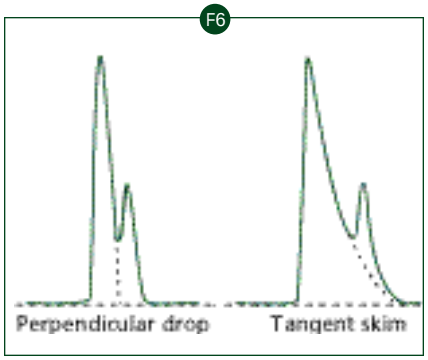

Figure 6: Quantification of unresolved peaks using perpendicular drop and tangent skim.

Each of these options should be enabled or disabled by a user within the method file.

Overlay of chromatograms: For a system with plotting options, a chromatogram overlay function should be available to enable you to compare results. This will be used to compare chromatograms from the same run sequence as well as chromatograms from different sources. The maximum number of chromatograms that can be overlayed should be known and the overlays are capable of offset by an amount determined by the user. Ideally, overlays from different run sequences (e.g., comparison of chromatograms over a time period) should be possible and have hidden lines removed. More sophisticated plots are possible if you have a data system and a diode array detector from the same vendor. Here the analysis of the diode array detection information can be interactively linked with the single wavelength data.

User-defined analytical run information: The system should be capable of collating user-defined parameters (e.g., height, area, ratios, concentrations etc.) for selected analytes from a sequence of runs. After collation, system-defined and/or user-defined statistical calculations will be performed on the data generated.

The type of calculations required should include mean, standard deviation, analysis of variance and possibly significance testing. Graphical representation of the data is vastly superior to tabulated figures and should be a requirement.

Reports and collation of results: Ideally, the report following an individual chromatogram should contain both elements that are user definable and those which are standard. This should enable the laboratory to customize their reports. The report writer for a CDS should have a wizard or equivalent to help the user build these reports for both ad hoc and routine uses.

Interfacing to Other Systems

Apart from acquiring data from chromatographic instruments, interfacing of a CDS should be considered for further analysis of data generated by the CDS (by interfacing I mean electronic transfer of data from the CDS rather than 'sneakernet' — floppy disk or manual input of data). Typical examples of interfacing are usually spreadsheets, word processors or laboratory information management systems (LIMS).

- The easiest form of interfacing is to a spreadsheet. In this instance, data are transferred from the CDS into the spreadsheet in a single direction for further data manipulation and reporting. Before starting this process, see if the CDS can undertake the calculations itself.
- Exporting a report directly into a word-processing package is another approach to help prepare the final report. Chromatograms only or the whole report can be exported, usually as an object, into the chosen word processor.
- Laboratory information management system: If a LIMS is planned or operational within the laboratory environment, two options exist for interfacing: a unidirectional upload of results from the CDS to the LIMS in a similar way to the spreadsheet or a two-way process. This latter involves the download of the LIMS worklist into the CDS, where it is incorporated into the sequence file. After analysis the results are uploaded into the LIMS for further collation with other results and final reporting.

This is an overview of what a CDS is — the life cycle and the key functions and problems. The next article in the series will look at the first stage of the life cycle: specifying and acquiring a CDS.

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