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Dynamic Data Exchange (DDE) with CARY OS/2 software

Application Note

Introduction

The increasing complexity of spectrophotometer data and the complex requirements of some GLP protocols has meant that chemists are making extensive use of spreadsheets for data manipulation and reporting.

This paper describes the use of DDE (Dynamic Data Exchange) to automate some of the procedures required to transfer data between applications so that this analysis can be simplified and automated.

Users wishing to conduct extensive manipulation of spectrophotometer data have conventionally been required to export the results at the end of the analysis using their spectrophotometer software, then re-import the data into their reporting program. DDE provides the opportunity to import data directly into another program without these lengthy procedures.

The DDE (Dynamic Data Exchange) facility in the Cary OS/2 software allows you to export data from the Cary OS/2 instruments directly into a DDE compatible spreadsheet or word processor while the data are/is actually being collected or displayed. In this case the Cary OS/2 software is referred to as the source application or server.

Typical examples of programs with DDE capability, are Microsoft Word for Windows, Excel for Windows, Lotus 123 for Windows or OS/2. All of these programs are referred to as the destination application or client program.



Procedures

To receive data from a Cary OS/2 spectrophotometer it is necessary to initiate communication through a series of commands, for example the string **CARY** | **DATA** ! **TYPE** creates a link to the host program to read plot data from the Cary program.

The data "TYPE" available to users are:

STATUS: This provides the current status messages from the Cary OS/2. These are the messages normally seen in the top line of the information bars in the Cary Base System and Applications.

ERROR: This transfers any errors that are displayed in the Cary Base System. These are normally displayed in the second line of the information bar.

PLOT: This provides the Abscissa, and Ordinate, and box identification generated by the Cary during the collection of a continuum. For example, during a wavelength scan, the wavelength in nanometres, the absorbance, and the continuum number and box number are sent from the Cary software in the form of a comma separated string. e.g. 447.59000,0.951832,0104.

This is interpreted as: Wavelength = 447.590000 Absorbance = 0.951832 Continuum number 01 in Box 04.

The PLOT data is read into the DDE link whenever a "RETRIEVE", "SHOW" continua, or a "COLLECT" or "READ" operation occur. Due to the nature of DDE function in Windows the computer may be totally occupied during the collect period.

When the PLOT data is sent to the client the data stream consists of the following components shown in Table 1.

Table 1. Cary DDE PLOT data

ltem	Format
File name	Current user\ Filename, X units,
Full path name	Drive\Path\Filename,Y units,
Ordinate range	Max-Min scaling of PLOT area,
Abscissa range	Max-Min Abscissa range, blank,
Data	Ordinate, Abscissa, scan
Continuing data	Ordinate, Abscissa, scan
End of data	"End of scan",, scan number-

If multiple cuvettes are being used with the multicell holder then the data stream consists of the first four lines of the above for each cell then the data stream for each cell reading as illustrated in Table 2.

Table 2. Cary DDE PLOT data for multicell operation

ltem	Format
File name	Current user\ Filename, scan
Full path name	Drive\Path\Filename, scan
Ordinate range	Max-Min scaling of PLOT area,
Abscissa range	Max-Min Abscissa range, scan
File name	Current user\ Filename, scan
Full path name	Drive\Path\Filename, scan
Ordinate range	Max-Min scaling of PLOT area,
Abscissa range	Max-Min Abscissa range, scan
Remaining cuvettes	
Data	Ordinate, Abscissa, 0101
Data	Ordinate, Abscissa, 0102
Remaining data for cuvettes	
End of data	"End of scan,,scan number box

IDLE: This displays the current readings in the Cary Base window abscissa and ordinate display, e.g. display. "550.000000,0.0123456789"

Example programs

The following examples illustrate using DDE in various spreadsheets. The resultant data handling is then limited by the capability of the spreadsheet. This formulated or processed data, diagrams, and graphs can then be linked by DDE or OLE to other compatible programs.

Microsoft Excel for Windows V4 or 5

The following cell entries shown in Table 3 will display data from the Cary OS/2 program.

The first column represents plain text to identify the data that will be displayed in the adjacent cell.

The second column represents the macro information that will collect data from the link to the Cary instrument. It is always necessary to start the Cary software before attempting to start a link. To start a DDE link, highlight the cell where you require the information to be input and type the commands shown below. When you press ENTER the system will immediately attempt to access the Cary system. If the system is present and active on the desktop the relevant information will be displayed. If no information is currently available "N/A" or if the Cary program is not active "#REF!" will be shown. These are Excel error messages and not text transferred from the Cary instrument. A series of DDE related messages will also be seen in the Cary status line. Changes in the Cary will be immediately reflected in the relevant cell.

Table 3. Cary DDE data types

Identification	Actual	Typical
Status messages	=Cary¦Data!Status	Scan 500-400 nm
Error messages	=Cary¦Data!Error	N/A
"Abs,Ord"	=Cary¦Data!Idle	553.6,0.1234
Plotted Abscissa Ordinate"	=Cary¦Data!Plot	553.6,0.1234,0101

As the data from the Cary instrument will be received in a stream, it is necessary to place the data in an array of cells. This is done be parsing the data stream as it is received.

It is necessary for a macro to be set that will activate a parsing macro when data is received in the application, once the above links are set, then changes in the links can be used to copy the data, parse the data stream and write it to an array of cells.

Macro for Excel 4 and 5

The EXCEL macro commands shown in Table 4 can be used to process the data supplied by the Cary.

The following macros show a typical application in gathering data from a plot into a three column table that can then be automatically incorporated into a graph. This graph can then be linked using OLE2 into Word for Windows version 6. The function "ON.DATA ("document_text","macro_text")" is used to detect changes in the range "document_text", when this occurs as information is received, then the parsing macro "macro_text" is run and the data is translated into rows of cells.

Note: range names are indicated in italics.

 Table 4. Excel 4 macro for Cary DDE

Range or Macro Names	Formulas	Comments			
Auto_Open_DDE	=ON.DATA("CARY DATA!P LOT","PLOT")	Change in "CARY PLOT" data			
		branch to PLOT			
		macro			
	=SELECT(SHEET1!\$A\$30)	GOTO cell A30			
	=RETURN()	EXIT			
PLOT					
PlotAbsOrd	=Cary Data!Plot	DDE Link			
CommaPos	=SEARCH(",",PlotAbsOrd)	Find first comma			
CommaPos2	=Search(CommaPos+1,",", PlotAbsOrd	Find second comma			
XVal	=MID(<i>PlotAbsOrd</i> ,1, <i>Comma</i> <i>Pos</i> -1)	Find Abscissa			
YVal	=MID(<i>PlotAbsOrd,CommaP</i> <i>os</i> +1,CommaPos2)	Find Ordinate			
ScanBox	=Right(PlotAbsOrd,4)	Find scan number and box number			
	=FORMULA(XVal)	Put Abscissa value in first cell			
	=SELECT(OFFSET(ACTIVE.C ELL(),0,1))	Move pointer to next column right			
	=FORMULA(YVal)	Put Ordinate value in cell			
	=SELECT(OFFSET(ACTIVE.C ELL(),0,1))	Move pointer to next column right			
	=FORMULA(Scanbox)				
	=SELECT(OFFSET(ACTIVE.C ELL(),1,-2))	Shift to next row first column			
	=RETURN()	Macro Return			
Auto_Close_DDE	=ON.DATA("PLOTDDE.XLM ")	Stop parsing routine			
	=RETURN()				

Excel 5 Visual Basic

Excel 5 for Windows enables users to create macros in Visual Basic. This provides an increase in capability of data presentation and versatility. It should be noted that Microsoft will only support Visual Basic in further releases of their products.

Table 5 illustrates a simple procedure to gather CARYdata into an array of cells.

The following parsing subroutine assumes there is a range called "PAO" in the active worksheet that contains the "CARY|DATA!PLOT" formula, and a cell named "FILE_NAME_START" to act as references.

Table 5. Visual Basic macro for Cary DDE

Visual Basic Code	Comment
Sub DDE START()	Macro subroutine name
Range("File Name Start").Select	Position cursor on active sheet
ActiveSheet.SetLinkOnData("CARY DATA!PLOT", "CODES")	On change in data do "Codes" macro
End Sub	
Sub Codes()	Macro subroutine name
On Error GoTo handle_errors	Error handling
cp = InStr(1, Range("PAO"), ",")	Get first comma location
cp2 = InStr(cp + 1, Range("PAO"), ",")	Get second comma location
xv = Left(Range("PAO"), cp - 1)	Get abscissa value
yv = Mid(Range("PAO"), cp + 1, cp2 - cp - 1)	Get ordinate value
scannum = Right(Range("PAO"), 4)	Get cell and scan number
Selection.Formula = xv	Past abscissa in active cell
Selection.Offset(0, 1).Activate	Move to next column
Selection.Formula = yv	Paste ordinate in active cell
Selection.Offset(0, 1).Activate	Move to next column
Selection.Formula = scannum	Past cell and scan number
Selection.Offset(1,-2).Activate	Reposition to first column and next row
Exit Sub	
handle_errors:	Error handling routine
Range("File_Name_Start").Select	
Endrun: End Sub	

The previous visual basic macro is a simplified routine to provide a three column layout of the data coming from the CARY instrument. Now the data is translated into rows and columns, further macros can be written to analyze or graph the data.

We have supplied a number of demonstration macros with the CARY OS/2 software which allow data to be translated, graphed and saved, together with creating extensive data arrays when multicell measurements are being taken.

VBXL5.XLS

This program is a universal routine where data are collected, parsed and displayed. It allows you to enter the number of cuvettes together with the SAT and DWELL times to ensure correct layout and ordering of the data.

VBKIN.XLS

This program is designed specifically for the Cary OS/2 Kinetics package. The incoming data stream is parsed and set out in rows and columns according to the individual cuvettes used in the multicell holder.

At the end of the analysis the data is automatically graphed and stored to an Excel file with the current sample name. Figure 1 (below) illustrates the presentation of data from the Cary Kinetics program into Excel 5.

	(inetics V		N	licrosoft Excel	- VBKIN.XLS	S		-	P
<u>F</u> ile <u>E</u> dit	<u>S</u> etup <u>C</u>	-	<u>File E</u> dit <u>V</u> iew	<u>I</u> nsert F <u>o</u> rπ	nat <u>T</u> ools	<u>D</u> ata	<u>W</u> indow		
		He	lp						l
DDE: Advise			A	В	С	D	E]
			Enter DWELL		2.0000				1
		6	time:		2.0000				
File		7	1						
_	·	<u> </u>		End DDE			7		
Setup		8	Start DDE	End DDE	្រ	raph Data	1		
7	Ĕ	9	Clear	Clear Data	1				
<u>Z</u> ero		ŤŬ		l	J				
	·		Plotted Abscissa,						
	J	11	Ordinate	#N/A					
	0.684		File Name	NDERS:KIN1	0101	ERS:KIN2		ER	
	0.004		Data Path Name	RS\KIN1.DAT	0101	KIN2.DAT		SEP	4
	Kinetice 1	14	Ordinate Range	0.00	10.20	0.00	10.20		q
	Kinetice (Abscissor Range	0.00	4.00	0.00	4.00		Q
	Kinetics (Kinetic Data	0.0889	1.604	0.1572	1.625	0	
	l'inchice 4			0.1056	1.603	0.1739	1.625	0	1
	Kinetice 9			1.0661	1.563	1.1339	1.589	1	1
	Kinetics (Kinetics 7			1.0828	1.562	1.1506	1.589	1	
_	Kinetice (20		2.0761	1.522	2.1611	1.549	2	
<u>C</u> alc	Kinetics 9			2.0928	1.522	2.1778	1.549	2	
	Kinetics .	22	4	3.0694	1.486	3.1378	1.518	3	
Print		23	{	3.0861	1.485	3.1544	1.518	3	1
rint a report		24	4	4.0633	1.451	4.1483	1.487	4	ł

Figure 1. Data layout in Excel VBKIN.XLS.

VBTHERM.XLS

This program is designed for use with the Cary OS/2Thermal application package. The data are collected, parsed and set out in rows and columns according to the number of cuvettes being used in the multicell holder. On completion the data are automatically plotted.

VBCONC.XLS

In this program the incoming data are parsed into rows and columns, then at the end a calibration graph is constructed from the data and a regression line is fitted to the data, the equation and fit parameters are then displayed.

VBSIMPLE.XLS

This program parses the incoming data and creates a plot of the data.

Lotus 1-2-3 for Windows Release 5

The Lotus macro(s) follow similar operation to those in EXCEL, allowing for the differences in nomenclature and protocols. To create the Link in LOTUS use the **EDIT LINK commands:**

Table 6. Lotus 123 DDE Link command for Cary

Link Name	Cary Plot (Option)
Application	CARY
Торіс	DATA
ltem	PLOT or IDLE or ERROR or
Format	TEXT
Update	AUTOMATIC

Table 7. Illustrates a simple set of macros to create a data array in Lotus 123

\A {GOTO}F1~ Position active cell {DDE-OPEN **Open Communications** "CARY"; "DATA"; NUMPLOT}~ place value of link in range "NUMPLOT" {DDE-ADVISE PLOTING; Do macro "PLOTING" if "PLOT"}~ PLOT value {DDE-CLOSE} **\PLOTING** {DDE-USE NUMPLOT}

{DDE-REQUEST ABSORD;"PLOT"}~ {LET Locate first comma "," COMMAPOS,@FIND(",",ABSORD,0)}~ separator in data string and insert in range COMMAPOS {LET Find length of data string and PLOTLENGTH,@LENGTH(ABSORD)}~ insert in range {LET Locate second comma COMMAPOS2,@FIND(",",ABSORD,CO separator in data string and MMAP0S+1)}~ insert in range COMMAPOS2 {LET ABSCISSOR,@VALUE Determine abscissa value and (@LEFT(ABSORD,COMMAPOS))}~ place in range ABSCISSA Insert ABSCISSA value in {LET @CELLPOINTER("ADDRESS"), ABSCIS column SA}~ {RIGHT}~ Move cursor right one column I FT Determine ordinate value and ORDINATE,@VALUE(@MID(ABSORD,(place in range ORDINATE COMMAPOS+1), (COMMAPOS2-COMMAPOS))) {LET @CELLPOINTER ("ADDRESS"), ORDINATE}~ column {DOWN}{LEFT}~

{DDE-UNADVISE "PLOT"}~ {DDE-CLOSE}~

Insert ORDINATE value in Move curser to previous column, next row. Exit routine. Close link

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