

Controlling the Agilent ChemStation Software for UV-visible Spectroscopy through Dynamic Data Exchange

Technical Note

Dynamic data exchange (DDE) is a fast and easy way to link independent applications that run on Microsoft[®] Windows[®] and NT[®] operating systems. The two DDE examples in this note show the capabilities of the Agilent ChemStation for UV-visible spectroscopy.

In the first example a small Visual Basic program communicates with the Agilent ChemStation application. In this DDE server situation the Agilent ChemStation can be remotely controlled and monitored by the Visual Basic client.

In the second application the Agilent ChemStation uses Microsoft Excel as a server for tabular data. Here an example is given of how the content of a table window can be transferred to an Excel spreadsheet.

Both examples can be used as a start-up for user applications.



Agilent Technologies

Introduction

Requirements

Special UV-visible spectroscopy applications often require special software. To avoid rewriting code and to simplify the generation of applications, this technical note gives examples of how to use the Agilent ChemStation software for UV-visible spectroscopy as a remotely controlled DDE server. This approach allows to use all features of Agilent Chem-Station and allows, for example, use Microsoft Visual Basic to generate the user interface and task control. The advantage of this approach is the free choice of the programming language and tools to create an application.

As well as Agilent ChemStation a second application is needed. The application that initiates communication is called a client and the application providing the service to the client is called a server. The programmability through macros and the built-in features of Agilent ChemStation mean it can be a client as well as a server in a DDE conversation. The examples in this note show a client and a server approach.

The server example uses a simple command line interface, programmed in Visual Basic 4.0, to control the Agilent ChemStation. Visual Basic is a tool that is often used to create user interfaces. Its graphical form designer offers many user interface elements which are able to communicate with the server application.

The second example shows the Agilent ChemStation in a client situation. The server used is Microsoft Excel. This example requires the advanced software for Agilent Chem-Station to generate macro programs. The application sends tabular data to Excel for further evaluation.

Principles of DDE

The DDE of the Microsoft Windows and NT operating systems allows to transfer information between standalone applications. The information interchange is organized in links. Applications can have multiple links. These links can be established in parallel to a single application or even different applications. Due to the direction of the transfer of information two types of links are available: a source link and a destination link. A source link sends information to the linked application and a destination link requests information from the linked application. In a typical DDE application both links are established at the same time: a source link to send information to the application and a destination link to receive feedback from the application.

Two examples are shown below. The first example uses the Agilent ChemStation as a server for a simple command line interface. The DDE communicaton is initiated by the command line window application.

In the second example a DDE link to Excel is established by the Agilent ChemStation. Excel is used as a server for results from the Agilent ChemStation.

Server example—from command line interface to Agilent ChemStation

Modern applications like Microsoft Word, Excel or Agilent ChemStation offer programmability in non-standard macro languages. These macro languages usually allow access to the entire functionality of the application. In addition, user macros can be written for specific tasks.

The first example, written in Visual Basic, is a remote command line interface to Agilent ChemStation. This remote command line interface allows to send all Agilent ChemStation macro commands to a Agilent ChemStation application. In the example code the Agilent ChemStation is automatically started in its offline version, if it's not already running.

The command line interface demonstrates a flexible way to control Agilent ChemStation. In a real application, buttons or other user interface elements could send the commands. Even complex sequences can be handled through this link. The command line window is shown in figure 1.

Remote Command Line to HP UV-Visible ChemStation

Print "Link OK!"

Figure 1 The remote command line window

Explanation

Three links are established by this Visual Basic application: a source link to a text box, and two destination links for the status information and possible error messages generated by the command entry.

The program listing is shown in table 1. The two destination links (Label2, Label3) are set to automatic links (vbLinkAutomatic). The link topics are properties of the label objects (Label2: HPUV-VISICPNOWAIT, Label3: HPUV-VISISYSTEM) as well as the link items (Label2:

_ErrMsg\$, Label3: Status). These links are handled automatically between the two applications. Whenever the status or the content of the error message variable

_ErrMsg\$ of the Agilent ChemStation server change, the caption of the linked labels are updated. The source link to send commands to Agilent ChemStation is handled manually. Only when the Enter key is pressed, is entire line of text send to Agilent ChemStation server through DDE. The link item is the Agilent ChemStation's macro command interpreter. In addition, the current status information is used to check whether the server is busy or not. If the server is busy, no command is send to the server and the text box is not cleared.

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IDLE

Table 1 Listing of the Visual Basic source code of the command line window application

VERSION 4.00 Begin VB.Form Form1 &H00C0C0C0& BackColor = = 4 'Fixed ToolWindow BorderStyle ClientHeight = 1620 ClientLeft = 1260 ClientTop = 1530 ClientWidth = 7110 BeginProperty Font \ {0BE35203-8F91-11CE-9DE3-00AA004BB851} = "MS Sans Serif" Name = 8.25 Size Charset = 700 = 0 'False = 0 'False = 0 Weight Underline Italic Strikethrough = 0 'False EndProperty ForeColor &H00000000& = 2025 Height = Icon = "Form1.frx":0000 1200 = Left "Form1" LinkTopic = 0 'False 0 'False MaxButton = MinButton = 1620 ScaleHeight = ScaleWidth = 7110 = 0 'False ShowInTaskbar -goT 1185 Width 7230 Begin VB.TextBox Text1 Height = 285 Left = 180 LinkTimeout = 5000 \ LinkTopic """HPUV-VIS|CPNOWAIT"" " = 1 TabIndex Text = "Print ""Link OK!""" 960 Тор = 6135 Width End Begin VB.Label Label3 2 'Center 1 'Fixed Single Alignment = BorderStyle = 285 Height Left = 6300 LinkItem "Status" = LinkTimeout = 500 LinkTopic = "HPUV-VIS|SYSTEM" TabIndex = 3 960 = Top Width 615 End Begin VB.Label Label2 BorderStyle = 1 'Fixed Single Height 255 180 Left "_ErrMsg\$" 3 'Notify LinkItem = LinkMode = LinkTimeout 500 = = "HPUV-VIS|CPNOWAIT" LinkTopic TabIndex = 2

Тор 720 Width 6735 End Begin VB.Label Labell Alignment = 2 'Center \ Caption _ "Remote Command Line to " + \setminus " HP UV-Visible ChemStation" BeginProperty Font \ {0BE35203-8F91-11CE-9DE3-00AA004BB851} Name = "MS Sans Serif" _ 12 Size = Charset 0 = 700 Weight 0 'False 0 'False Underline = Italic = 'False Strikethrough = 0 EndProperty 375 Height Left = 180 TabIndex = 0 Тор = 240 Width = 6735 End End Attribute VB_Name = "Form1" Attribute VB_Creatable = False Attribute VB_Exposed = False Private Sub Form Load() On Error GoTo LoadApplication Label2.Caption = "" ' clear error Label3.LinkMode = vbLinkAutomatic ' initiate link status Exit Sub LoadApplication: ' trap application not On Error GoTo O ' started, reset trapping h = MsgBox \setminus ("Starting UV-Visible Chemstation", 65) ' allow user to exit If h = 1 Then h = \ Shell("C:\HPCHEM\SRELEASE\HPUV-VIS 1", 4) Call Sleep(90000) ' wait 90 seconds ' Start ChemStation. Else End End If ' continue Resume End Sub Private Sub Form Unload(Cancel As Integer) Text1.LinkMode = vbNoneLabel2.LinkMode = vbNone Label3.LinkMode = vbNone

```
End Sub
Private Sub Label2 Change()
         h = Len(Label2.Caption)
         If h > 2 Then
             Label2.BackColor = &HFF&
         End If
End Sub
Private Sub Label2 LinkOpen(Cancel As Integer)
      Label2.Caption = "" ' reset
End Sub
Private Sub Label3 Change()
     If InStr(1,Label3.Caption,"BUSY") > 0 Then
          Label3.BackColor = &HFF0000
Label3.ForeColor = &HFFFFFF
     Else
          Label3.BackColor = &HFF00&
          Label3.ForeColor = &HO&
     End If
End Sub
Private Sub Label3 LinkOpen(Cancel As Integer)
       Label3.Caption = "" ' reset
End Sub
Private Sub Text1_KeyPress(KeyAscii As Integer)
                               ' Enter ?
If KeyAscii = 13 Then
   Label2.Caption = ""
                              ' reset
   Label2.BackColor = &HC0C0C0
   If InStr(Label3.Caption, "IDLE") > 0 Then
    If Text1.LinkMode = vbNone Then
                         ' not yet established ?
            Text1.LinkTopic = \
                              "HPUV-VIS|CPNOWAIT"
            Text1.LinkMode = vbLinkManual
        End If
        Text1.LinkExecute Text1.Text
                         ' Set link item.
        Text1.Text = "" ' reset command line
   Else
                         ' cannot execute
       Beep
   End If
End If
End Sub
```

Discussion

The command line window example in Visual Basic shows the principle of how Agilent ChemStation can be used as a server to a user application. To help customizing these special applications, a few useful macro commands are listed in table 2.

When using these macros care must be taken of the correct order and appropriate status of the spectrophotometer and the application. For example, before any sample or standard measurement, a blank must be measured. Or, in quantitative analysis, the system must be calibrated before samples can be analyzed. The simplest way to achieve such conditions is to set up the method according to the applications requirements.

These macros use the current parameter of the method. In addition to the system macros, user macros can be created to further simplify the programming effort.

Table 2 Example macros for selected tasks (S = standard tasks, A = advanced, D = dissolution)

Task	Commands	Application
Blank measurement	MeasureBlank()	S,A,D
Sample measurement	MeasureSample()	S,A,D
Standard measurement	MeasureStd()	S,A,D
Auxilliary measurement	MeasureAux()	S,A,D
Control measuement	MeasureControl()	
Change application	zzswGUISwitchMode " <mode name="">"</mode>	all
Disable userinterface	busy=1	S,A,D
	zzswCheckButtons	
	MenuDelete	
	zzDisableFKeys	
Enable userinterface	zzBaseMenu	S,A,D
	zzStartMenu	
	zzGenericMenuPart "UserContrib"	
	busγ=0	
	zzswCheckButtons	
Load samples	LoadSamples	S,A,D
Load standards	LoadStandards	S,A,D
Load auxiliary	LoadAuxiliary	S,A,D
Save samples	SaveAsSamples	S,A,D
Save standards	SaveAsStandards	S,A,D
Print results report	zzrpPrint("Results")	A,D
View results report	zzrpPrint("Results","SCREEN")	A,D
Print method	zzrpPrint("Method")	A,D
View method	zzrpPrint("Method" ,"SCREEN")	A,D
Load method	LoadMethod()	S,A,D

Client example—transfer of tabular Agilent ChemStation data to Excel

This Agilent ChemStation macro uses Excel as a server. Agilent ChemStation initiates the DDE conversation and transfers data to spreadsheets. In the example macro code shown in table 3, a simple user interface was added to check and demonstrate the macros. The data of a table displayed in Agilent ChemStation windows can be transferred to Excel using the **Export** menu's **Export** selected table to Excel command. The macros used with this example can be integrated into automated sequences.

Explanation

To transfer the data of an existing table only two macro functions are required: DDE_Excel_Init() and SendTable().

The macro function DDE_Excel_Init() establishes a DDE link to the specified spreadsheet. In addition this macro function starts an Excel session, if Excel was not already running. The path required to start Excel is stored in Agilent ChemStation's Features.ini file. Either a text editor or the comand SetPrivateProfileString can be used to set a valid Excel path.

Table 3 Listing of macro file DDE_Excel.MAC

```
****
  FILE
     DDE Excel.MAC
  DESCRIPTION
     Macros for sending tables to MS-Excel an spreadsheet.
  Version Rev 1.0 23.11.98 Thomas Klink
     EXPORTS
  *****
  RunExcelMacro SysChannel, Send run macro instruction to MS-Excel
              MacroName$,
                            Spreadsheet via SysChannel
              [SpreadSheet$]
  MenuExport
                            Add entry to Export menu
  ExportSelectedTable
                            Get and check for valid selection
                             of table and export to MS-Excel
              [SpreadSheet$] Initialize transfer to MS-Excel
RegObj$,TabName$, Send table column to MS-Excel
  DDE Excel Init [SpreadSheet$]
  SendColumn
                             spreadsheet
              ColumnName$,
              DDE_Chan,StartRow,
              Col
  SendTable
            RegObj$,TabName$, Send table to MS-Excel spreadsheet
              DDE Chan,[StartRow],
              [StartCol]
  SendVal
              Val,DDE Chan,
                            Send value to spreadsheet
              Row,Col
  SendText
              Text$,DDE Chan,
                           Send string to spreadsheet
              Row,Col
  MACROS
        *****
                        ******
NAME RunExcelMacro
  Parameter SysChannel
                                   ! active DDE channel
  Parameter MacroName$
                                    ! run macro
                   Default ""
                                  ! active spreadsheet
  Parameter SpreadSheet$
  DESCRIPTION
     Send run macro instruction to MS-Excel Spreadsheet via SysChannel
 RETURN
   True (1), no error, False(0), error
  *******
                           ****
  On Error Return 0
  If SpreadSheet$ = "" then
```

```
DDEExecute SysChannel, "[run("""+MacroName$+""")]"
    else
       DDEExecute SysChannel,"[run(""+SpreadSheet$+"!"+MacroName$+""")]"
   Endif
    Return 1
EndMacro
Name MenuExport
   DESCRIPTION
       Add entry to Export menu
   RETURN
       None
      MenuAdd "E&xport",,"SEPARATOR"
       MenuAdd "E&xport", "Export selected Table to Excel", ExportSelectedTable
EndMacro
NAME ExportSelectedTable
   DESCRIPTION
      Get and check for valid selection of table and export to MS-Excel
  RETURN
    None
  *******
                  *****
   LOCAL Chan, LastRow, Win, x
   LOCAL RegObj$, TabName$, C$
   Win = ActiveWindow()
                                                 ! get current selection
    IF Win = 0 THEN
                                                  ! check
       PRINT #2, "Select/activate a table window!" ! nothing selected
       RETURN
   ENDIF
   L$ = TabText$(_CONFIG[1],"WINDOW",Win,"Command")! get command to restore
    if Len(L\$) > 0 then
                                                 ! not empty ?
       C$ = zzrpGetNextParam$("L$")
                                                ! get command keyword
       if C$="EdTab" OR C$="edtab" OR C$="EDTAB" then
           RegObj$ = zzrpGetNextParam$("L$") ! ignore first (WinNr)
RegObj$ = ConvertText$("TRIM",zzrpGetNextParam$("L$")) ! get RegObj
TabName$ = ConvertText$("TRIM",zzrpGetNextParam$("L$")) ! get TabName
           Chan = DDE Excel Init()
                                                 ! open DDE communication
           Print "Sending table "+RegObj$+","+TabName$+" to Excel" ! message
           LastRow = SendTable(RegObj$, TabName$, Chan)
                                                               ! send table
           DDEterminate Chan
                                                ! close DDE channel
           Return
                                                  ! ready!, exit
       EndIf
    EndIf
    x = Alert("Could not export:"+Chr(13)+Chr(10)+
              L$+Chr$(13)+Chr$(10)+"to Excel!", 3, "Export to Excel")
ENDMACRO
```

```
. *****
Name DDE Excel Init
  Parameter SpreadSheet$ Default "" ! active spreadsheet
   DESCRIPTION
       Initialize transfer
   RETURN
! Channel, -1 = Error
                           Local Chan, h, i, x
    Local Topics$, Topic$
    On Error Goto StartExcel
    x = 0
Again:
    Chan=DDEinitiate("Excel", "System")
    DDErequest Chan, "topics", Topics$
    DDETerminate Chan
    If SpreadSheet$ = "" then
        Topics$ = zzrpReplace$(Topics$, Chr$(9), "|")
        i = Instr(Topics$,"|System")
        Topics$ = Topics$[1:i-1]
        Topic$ = SubString$(Topics$,1)
        RemoveDialog ExportToExcel
        BeginDialog ExportToExcel, 50, 40,120, 80,"Send selected table to Excel"
StaticText 10, 12, 80, 20, "Destination sheet:"
ComboBox 10, 25,100, 80, Topic$
        OkButton 10, 55, 40, 16
CancelButton 70, 55, 40, 16
        EndDialog
        h = ShowDialog(ExportToExcel)
        RemoveDialog ExportToExcel
        if h = 0 then
                                                          ! cancel ?
            Return -1
                                                           ! exit
        EndIf
    Else
       Topic$ = SpreadSheet$
    EndIf
    Chan=DDEinitiate("Excel", Topic$)
    DDEexecute Chan,"[activate("""+Topic$+""")]"
    Print "Connecting to " + Topic$
Return Chan
StartExcel:
    If \_Error = 41330 and x = 0 then
                                                     ! Excel not running
        x = 1
                                                     ! first attempt
        Print "Trying to start Excel..."
                                                   ! display message
        ExcelPath$ = PrivateProfileString$("ExportToExcel", "ExcelPath", \
        _ExePath$+"features.ini","C:\MSOffice\Office")
ExecNoWait ExcelPath$ + "\Excel.exe"
        Sleep 10
        Goto Again
```

```
Else
        On Error
                                                       ! reset error trapping
        If _ErrCmd$ = "ExecNoWait" Then
            x = Alert("Could not start Excel!"+Chr(13)+Chr(10)+
                       "Path : "+ExcelPath$+" correct?"+Chr$(13)+Chr$(10)+\
                       "Use 'Configure Excel path...' command to set."\
                       ,3,"Export to Excel")
        Else
           x = Alert("Error in macro DDE_Excel_Init: "+_ErrMsg$,3,"Export to Excel")
        EndIf
        Return -1
                                                      ! could not open channel
    EndIf
EndMacro
•
NAME SendColumn
    Parameter RegObj$
                                                      ! table register object
    Parameter TabName$
                                                      ! table name
    Parameter ColumnName$
                                                      ! column name
    Parameter DDE_Chan
                                                      ! active DDE channel
    Parameter StartRow
                                                      ! spreadsheed start row
    Parameter Col
                                                      ! spreadsheet column
    DESCRIPTION
        Send table column to Spreadsheet via DDE_Chan
  RETURN
      None
             | * * * * * * * * * *
    Local C$, H$,X$
    Local h,i,t,x
                                                     ! initialize column id
    C$ = "c"+Val$(Col)
    DDEpoke DDE Chan,"r"+val$(StartRow)+C$,ColumnName$
    Evaluate "h = TabHdrVal("+RegObj$+",TabName$,""NumberOfRows"");"+\
    "t = TabColType("+RegObj$+",TabName$,ColumnName$)"
    If t = 0 then
                                                       ! string ?
        Evaluate "For i = 1 to h;"+ 
                     "X$ = TabText$("+RegObj$+",TabName$,i,ColumnName$);"+\
"DDEpoke DDE_Chan,""r""+Val$(StartRow+i)+C$"+",X$;"+\
                  "Next i"
    EndIf
    If t > 0 then
                                                       ! number ?
        Evaluate "For i = 1 to h;"+ 
                      "x = TabVal("+RegObj$+",TabName$,i,ColumnName$);"+\
                      "if x > -1.7977e+308 then;"+\
                           "ddepoke DDE_Chan,""r""+Val$(StartRow+i)+C$"+\
                                             ",SPrintF$(x,""%2.21g"");"+\
                      "else;"+\
                          "ddepoke DDE_Chan,""r""+Val$(StartRow+i)+C$"+\
",""***"";"+\
                      "endif;"+\
                   "Next i"
    EndIf
EndMacro
```

```
*************
NAME SendTable
   Parameter RegObj$
                                             ! table register object
                                             ! table name
   Parameter TabName$
   Parameter DDE Chan
                                             ! active DDE channel
   Parameter StartRow Default 1
                                            ! spreadsheed start row
   Parameter StartCol Default 1
                                            ! spreadsheed start column
   DESCRIPTION
      Send table to Spreadsheet via DDE Chan
  RETURN
    True (1), no error, False(0), error
  *****
   Local ColumnName$
   Local h,Row,Col
   Row = StartRow ! start row in spreadsheet
DDEpoke DDE_Chan,"r"+Val$(Row)+"c"+Val$(StartCol),"Table: "+RegObj$+","+TabName$
   Row = Row + 2
                                              ! increment row
   Col = 1
                                              ! start with first column
   Evaluate "Repeat;"+\
               "ColumnName$=TabColName$("+RegObj$+",TabName$,Col);"+\
               "If ColumnName$ <> """" then;"+\
                   "SendColumn RegObj$,TabName$,ColumnName$,DDE_Chan,Row,StartCol+Col-1;"+\
                   "Col=Col+1;"+\
               "EndIf;"+\
           "Until ColumnName$ = """";"+\
           "Row = Row + TabHdrVal("+RegObj$+",TabName$,""NumberOfRows"") + 2"
   Return Row
EndMacro
•
NAME SendVal
   Parameter Val
                                              ! value to transfer
   Parameter DDE Chan
                                              ! open DDE channel
                                              ! spreadsheed row
! spreadsheed column
   Parameter Row
   Parameter Col
   DESCRIPTION
      Send value to spreadsheet via DDE Chan
  RETURN
    None
       DDEpoke DDE Chan, "r"+Val$(Row) + "c"+Val$(Col), Val$(Val)
EndMacro
```

!***	*******	***************************************	* * *	* * * * * * * * * * * * * * * * * * * *			
NAME	SendText						
	Parameter	Text\$! :	string to transfer			
	Parameter	DDE_Chan	! 0	open DDE channel			
	Parameter	Row	!	spreadsheed row			
	Parameter	Col	!	spreadsheed column			
1	DESCRIPTION						
!	Send string to spreadsheet via DDE_Chan						
!							
!							
! RETURN							
!	! None						
* * * * * * * * * * * * * * * * * *							
	DDEpoke DDE_Chan,"r"+Val\$(Row)+"c"+Val\$(Col),Text\$						
EndMa	acro						

For example, the path C:\MSOffice\Office can be set using:

```
SetPrivateProfileString
"ExportToExcel",\
"ExcelPath",
"C:\MSOffice\Office",\
ExePath$+"Features.ini"
```

After successful completion of the DDE_Excel_Init macro function a DDE channel number is available for the data transfer. Even multiple channels in parallel can be used to send tables to different spreadsheets.

The information of an entire table is transferred by the 'SendTable' macro function. Only the register where the table resides, the table name and the DDE transfer channel have to be specified to send all table data. Optionally the starting row and column can be specified. If multiple tables shall be transferred, the return value of the SendTable function provides the starting row for the next table.

If only certain columns of a table shall be transferred, the macro command SendColumn can be applied. This macro transfers a single column only. In addition to the parameters of the SendTable function, the column name, the start row index and the column index have to be specified.

For other information the two macro commands SendVal and SendText can be used. They allow to set the content of a single spreadsheet cell with a numerical value or a text string.

To use the functionality of Excel, the RunExcelMacro function is provided. The macro function allows to execute macros created with a spreadsheet. Assuming you recorded your first Macro1 with the Excel macro recorder, you can execute this macro using:

Print RunExcelMacro (DDE_Chan,"Macrol")

This command requires the Excel Macro1 to be available with the currently-used DDE channel (DDE_Chan).

To release a DDE channel, the command DDE terminate is available.

Conclusion

References

The three applications Microsoft Visual Basic, Microsoft Excel and the Agilent ChemStation for UV-Visible spectroscopy have been used to demonstrate how independent applications can be linked for remote control and data interchange. The examples given are meant as a starting point for creation of complex applications by linking specialized applications together. DDE is not limited to these applications only. Even two instrument sessions in the Agilent ChemStation world can be linked—spectral data can be sent from a chromatographic run to a spectroscopy session where they can be further analyzed.

A Macro Programming Guide is provided in Adobe® Acrobat[®] Portable Data Format (PDF) with the Advanced Agilent ChemStation software for UV-Visible spectroscopy. It is a good starting point to write macros for Agilent ChemStation. The command syntax is available in Agilent ChemStation help files. Macro examples are provided with Agilent ChemStation family software products disk. In the directory Ucl\, examples for the various Agilent ChemStation products can be found.

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Publication Number 5968-3616E



Agilent Technologies