

Standard Operating Procedure

Task: Using OceanView's File Writer and Importing Data to Excel

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Background:

- When investigating kinetics or intermediates in reactions by UV-Vis, it is often convenient to set up a File Writer for OceanView to automatically collect spectra. When the entire spectrum is collected, each time point is saved in a separate tab-delimited text file. A macro to import these files into Excel is included.

Training Requirements:

- Lab Safety Training
- UV-Vis Training

Potential Hazards:

- Hazards associated with a UV-Vis experiment

Special PPE Requirements:

- None

Materials Needed:

- Materials for your experiment
- OceanView
- Excel

Procedure:

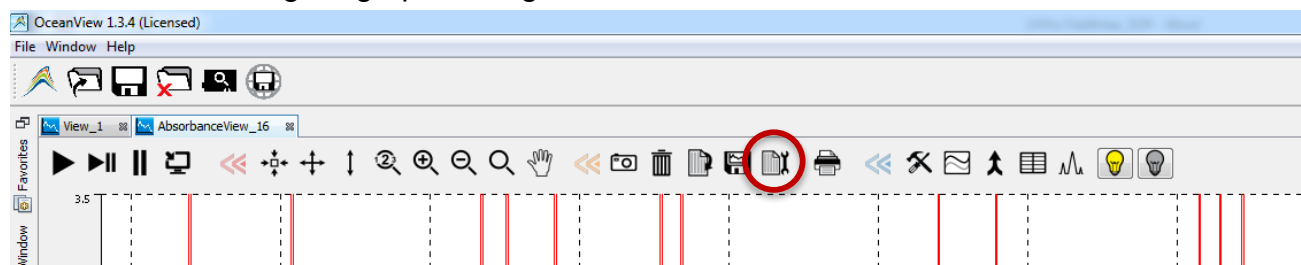
This SOP includes Setting up a File Writer, Making a Strip Chart, and Importing Data to Excel.

- The file writer example is shown for recording full absorbance spectra, but an analogous file write can be configured for any tab in OceanView. For example, a single wavelength can be monitored by making a strip chart and using a file write on that tab.
- Importing Data to Excel is specific to full absorbance spectra from OceanView.

Setting up a File Writer

1. Set up an absorbance spectrum as usual. Note: it's good practice to configure your file writer before running your sample of interest and ensure that the data is saving as expected. If OceanView is not close, the same file writer configuration can be used multiple times.

2. Select “configure graph saving”



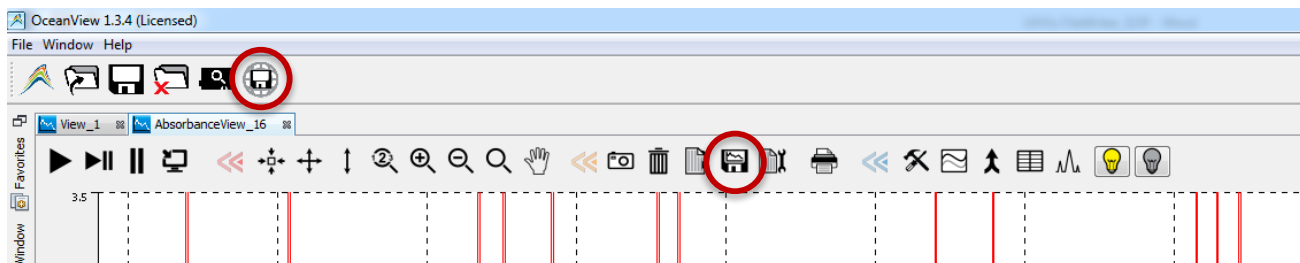
3. Click “Yes”

4. Fill out the form to save spectra with desired frequency (e.g. 30 s below). The Writer can be configured to stop automatically after a given amount of time or scans, or can be manually ended. Make a new directory to save files to. Use “Tab separated with Headers.”

The screenshot shows the 'Algorithm Parameter Controls' dialog box, specifically the 'File Writer_11 (File Writer)' section. The 'Input A' is set to 'Aggregate_10'. The 'Save Options' tab is active, showing options for saving scans. The 'File Options' tab is also visible, showing options for saving to a directory and file format. The 'Save Options' section includes radio buttons for 'Save every scan:', 'Save after every:', 'Between saved scans, wait at least:', and 'Save the first available scan every:'. The 'Save the first available scan every:' option is selected, with a value of 30 seconds. The 'File Options' section includes a 'Save to Directory:' field with a path, a 'File Format:' dropdown set to 'Tab separated with Headers', a 'Padding Digits:' field set to 5, a 'BaseName:' field, and a 'Preview example:' field showing 'viewdata01234.txt'. There are 'Apply' and 'Exit' buttons at the bottom.

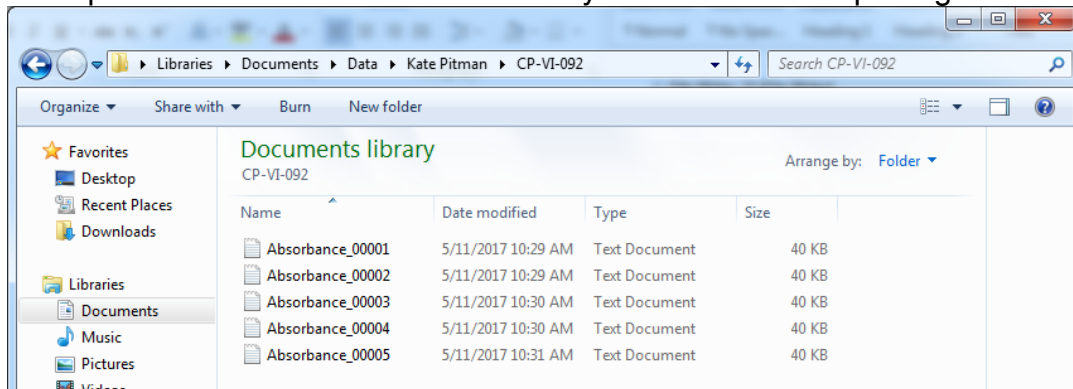
5. Click “Apply” and “Exit”

6. Select either “Start all file writers” or “Save graph to file/files” to begin recording data.



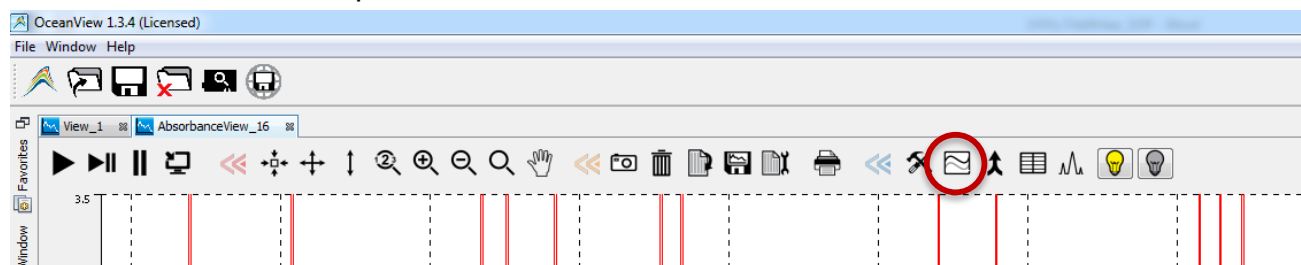
Note: multiple types of file writers can be configured at once. You could, for example, record single wavelength data (below) while recording the entire spectrum. If multiple file writers are configured, use “start all file writers” in the top left corner.

7. The spectra are saved to the set directory. See below for importing into Excel.

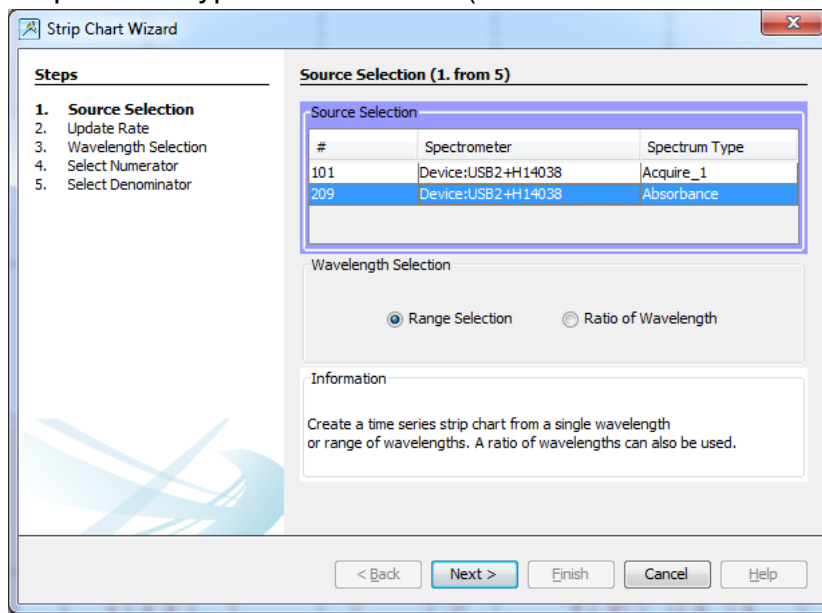


Making a Strip Chart

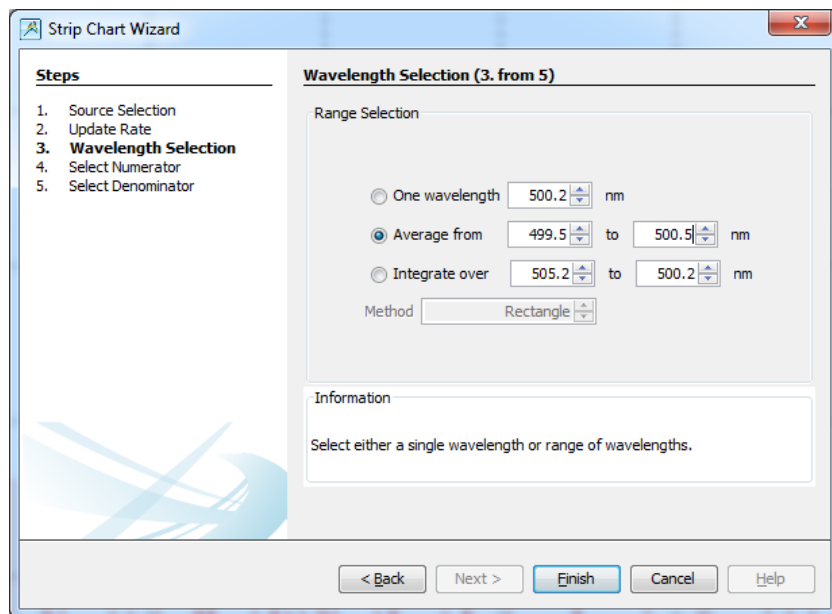
1. Select “create strip chart”



2. Select Spectrum Type = Absorbance (101 is the instrument's raw data). Click Next

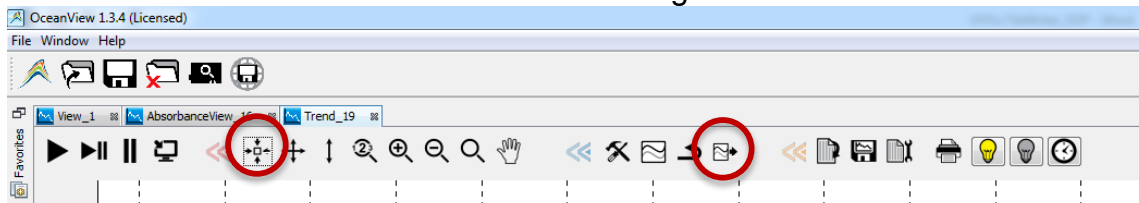


3. Select refresh rate and when to stop recording (typically update after every scan and never stop) Note: this does not save the data. It just displays it to the strip chart.
4. Select Wavelength to monitor. Click Finish.



5. A new tab appears with the trend line.

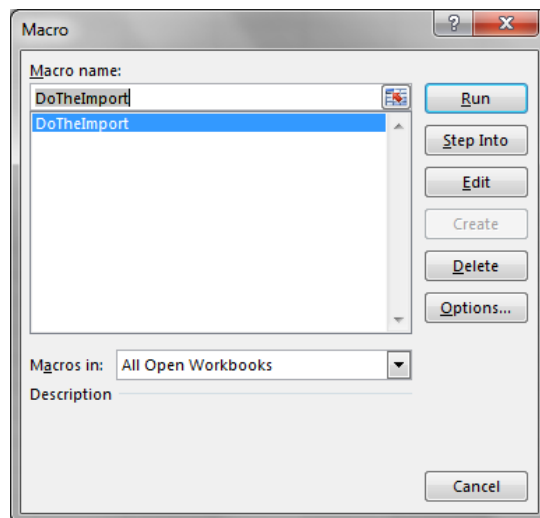
- The screen may need to be recentered. “Automatically scroll the trend line” will follow as new data is collected. A FileWriter can be configured to save the trend line as above.



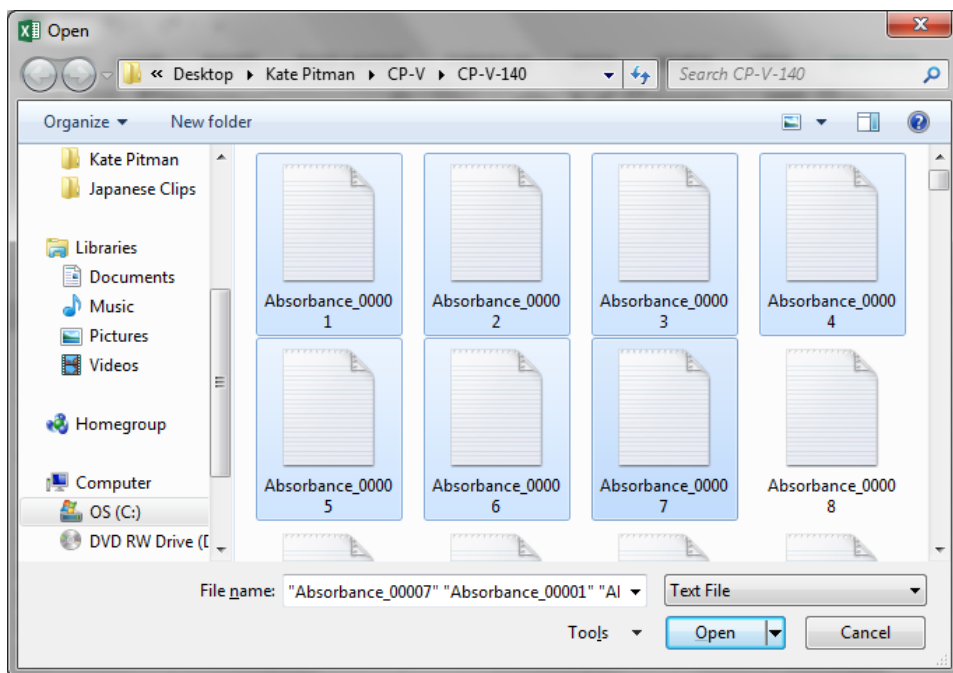
- Note: the trend line only saves data temporarily. As a new data point is collected, the oldest data point is deleted.

Importing Data to Excel

- Note: the macro to do the import is not robust. If you give it an input it doesn't expect, it can't handle it.
- On the desktop of the desktop computer in folder “File Writer Import,” open “CP-VI-092.xlsx.” If anything is in the notebook, delete it.
- Make sure cell A1 is selected.
- Under View>Macros>View Macros
- From the Macro screen, run “DoTheImport”



6. Select the files you want to import. They must be OceanView txt files with Headers. Use Shift and Ctrl multiple files. Note: if you have more than 255 files, Excel cannot plot them all together (and this will be very slow). For best results, divide amongst multiple Excel sheets.

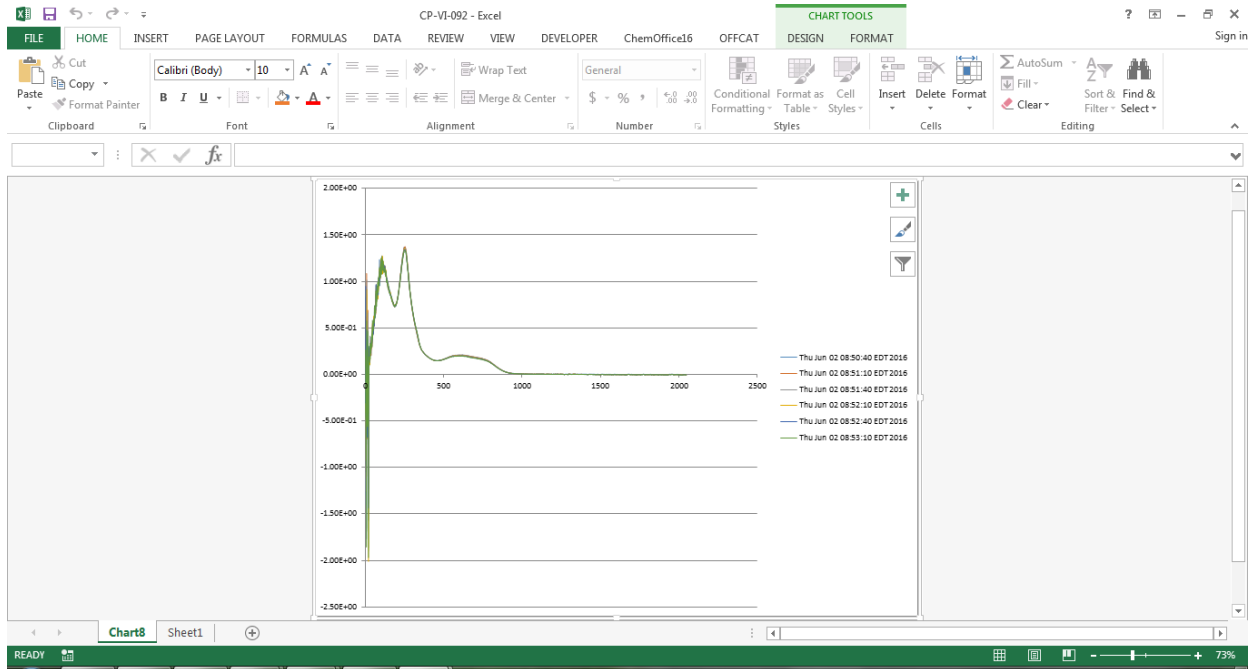


7. Select open.
8. The files will be imported into Excel. The wavelength column will only be copied from the first file and is in Column A. Row 1 contains the time each spectrum was recorded.

A screenshot of an Excel spreadsheet titled 'CP-VI-092 - Excel'. The ribbon shows 'FILE', 'HOME', 'INSERT', 'PAGE LAYOUT', 'FORMULAS', 'DATA', 'REVIEW', 'VIEW', and 'DEVELOPER'. The 'HOME' tab is active, showing options for Clipboard, Font, Alignment, and Number. The spreadsheet has columns A through J and rows 1 through 10. Row 1 contains timestamps for each column. Rows 2 through 10 contain numerical data in scientific notation.

	A	B	C	D	E	F	G	H	I	J
1		Thu Jun 02 08:50:40 EDT 2016	Thu Jun 02 08:51:10 EDT 2016	Thu Jun 02 08:51:40 EDT 2016	Thu Jun 02 08:52:10 EDT 2016	Thu Jun 02 08:52:40 EDT 2016	Thu Jun 02 08:53:10 EDT 2016	Thu Jun 02 08:53:40 EDT 2016		
2	1.8996E2	-19.508E-2	2.08E-02	2.02E-02	-2.97E-01	-3.04E-01	2.62E-01	2.47E-01		
3	1.90E+02	-1.95E-01	2.08E-02	2.02E-02	-2.97E-01	-3.04E-01	2.62E-01	2.47E-01		
4	1.91E+02	-1.95E-01	2.08E-02	2.02E-02	-2.97E-01	-3.04E-01	2.62E-01	2.47E-01		
5	1.91E+02	0.00E+00	6.16E-01	1.52E-04	-1.07E-01	9.46E-01	0.00E+00	0.00E+00		
6	1.91E+02	3.70E-01	2.43E-01	-6.31E-01	-4.18E-01	0.00E+00	-4.72E-01	-4.65E-01		
7	1.92E+02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-3.81E-01	0.00E+00	0.00E+00		
8	1.92E+02	-1.40E+00	-8.35E-01	-1.25E+00	-1.04E+00	-1.04E+00	-9.18E-01	0.00E+00		
9	1.93E+02	0.00E+00	-1.23E+00	0.00E+00	-2.11E-01	-8.86E-01	0.00E+00	0.00E+00		
10	1.93E+02	-1.77E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	-1.85E+00	0.00E+00		

9. A separate worksheet contains the data as a chart.



10. Save the Excel file under a new name. File > Save As > Your File Name. Save As type can be set to “Excel Workbook” rather than “Macro Enabled Workbook”

References and Related SOPs:

- Ocean Optics UV Vis_SOP

Appendix A. Code for import

```

Sub DoTheImport()
' This prompts the user for an array of FileName, assumes the
' separator is a tab, and then calls the appropriate sub to
' import the file. A sub is then called to make a chart.
    Dim FileName() As Variant
    Dim Sep As String
    Dim Index As Integer
    FileName() = Application.GetOpenFilename(FileFilter:="Text File (*.txt),*.txt",
MultiSelect:=True)
    If Not IsArray(FileName) Then
        .....

        ' user cancelled, get out
        .....

        Exit Sub
    End If
    'Defining the file at tab delimited
    Sep = vbTab
    'Sep = Application.InputBox("Enter a separator character.", Type:=2)
    'If Sep = vbNullString Then
        .....

        ' user cancelled, get out
        .....

        'Exit Sub
    'End If
    'Debug.Print LBound(FileName) & UBound(FileName)
    ImportFirstTextFile FName:=CStr(FileName(1)), Sep:=CStr(Sep)
    'Steps through the array of files to import
    For Index = 2 To UBound(FileName)
        ImportNextTextFiles FName:=CStr(FileName(Index)), Sep:=CStr(Sep), Col:=(Index + 1)
    Next
    Rows(2).Delete
    CreateChart traces:=(UBound(FileName))
End Sub
.....

```

```

Public Sub ImportFirstTextFile(FName As String, Sep As String)
' This imports the first file (including wavelength) into Excel.
Dim RowNdx As Long
Dim ColNdx As Integer
Dim TempVal As Variant
Dim WholeLine As String
Dim Pos As Integer
Dim NextPos As Integer
Dim SaveColNdx As Integer

```

```
Application.ScreenUpdating = False
'On Error GoTo EndMacro:
```

```
SaveColNdx = ActiveCell.Column
RowNdx = 2
```

```
Open FName For Input Access Read As #1
```

```
While Not EOF(1) 'steps through the lines of the file
```

```
    Line Input #1, WholeLine
```

```
    If Right(WholeLine, 1) <> Sep Then
```

```
        WholeLine = WholeLine & Sep
```

```
    End If
```

```
    'This ifThen is putting the time in the first cell
```

```
    If InStr(WholeLine, "Date") > 0 Then
```

```
        Cells(1, SaveColNdx + 1).Value = Mid(WholeLine, InStr(WholeLine, "Date") + 6,
InStr(WholeLine, "User") - InStr(WholeLine, "Date") - 6)
```

```
    End If
```

```
    'for whatever reason the first data point got caught in the header. This pulls it out.
```

```
    If RowNdx = 3 Then
```

```
        Cells(3, SaveColNdx).Value = Mid(WholeLine, InStr(WholeLine, "<<<<<<") + 5, 9)
```

```
        Cells(3, SaveColNdx + 1).Value = Mid(WholeLine, InStr(WholeLine, vbTab))
```

```
    ElseIf RowNdx > 3 Then
```

```
        ColNdx = SaveColNdx
```

```
        Pos = 1
```

```
        NextPos = InStr(Pos, WholeLine, Sep)
```

```
        While NextPos >= 1
```

```
            TempVal = Mid(WholeLine, Pos, NextPos - Pos)
```

```
            Cells(RowNdx, ColNdx).Value = TempVal
```

```
            Pos = NextPos + 1
```

```
            ColNdx = ColNdx + 1
```

```
            NextPos = InStr(Pos, WholeLine, Sep)
```

```
        Wend
```

```
    End If
```

```
    RowNdx = RowNdx + 1
```

```
Wend
```

```
EndMacro:
```

```
On Error GoTo 0
```

```
Application.ScreenUpdating = True
```

```
Close #1
```

```
End Sub
```

```
.....
```

```
Public Sub ImportNextTextFiles(FName As String, Sep As String, Col As Integer)
```

```
    ' This imports all following text files (only the 2nd column)
```

```
    Dim RowNdx As Long
```

```
Dim TempVal As Variant
Dim WholeLine As String
Dim Pos As Integer
Dim SaveColNdx As Integer
```

```
Application.ScreenUpdating = False
'On Error GoTo EndMacro:
```

```
RowNdx = 2
```

```
Open FName For Input Access Read As #1
```

```
While Not EOF(1)
```

```
    Line Input #1, WholeLine
```

```
    'Having this in here was leading to a tab at the end of the value so Excel read it as text.
```

```
    'If Right(WholeLine, 1) <> Sep Then
```

```
        WholeLine = WholeLine & Sep
```

```
    'End If
```

```
    'This ifThen is putting the time in the first cell
```

```
    If InStr(WholeLine, "Date") > 0 Then
```

```
        Cells(1, Col).Value = Mid(WholeLine, InStr(WholeLine, "Date") + 6, InStr(WholeLine,
"User") - InStr(WholeLine, "Date") - 6)
```

```
    End If
```

```
    Pos = InStr(1, WholeLine, Sep)
```

```
    TempVal = Mid(WholeLine, Pos + 1)
```

```
    Cells(RowNdx, Col).Value = TempVal
```

```
    'Debug.Print (TempVal)
```

```
    RowNdx = RowNdx + 1
```

```
Wend
```

```
EndMacro:
```

```
On Error GoTo 0
```

```
Application.ScreenUpdating = True
```

```
Close #1
```

```
End Sub
```

```
.....
```

```
Sub CreateChart(traces As Integer)
```

```
    'PURPOSE: Create a chart with all traces from Ocean view data
```

```
    If traces <= 255 Then
```

```
        Dim rng As Range
```

```
        'this assumes that the data starts in A1 and is coming from OceanView with 2048 data
points
```

```
        Set rng = ActiveSheet.Range(Cells(1, 1), Cells(2048, traces))
```

```
        Charts.Add
```

```
        ActiveChart.ChartType = xlXYScatterSmoothNoMarkers
```

```
    ActiveChart.SetSourceData Source:=rng, PlotBy:=xlColumns  
End If  
End Sub  
.....
```