Workflow in CasaXPS

The batch processing options described herein are available in CasaXPS version 2.3.27PR7.0

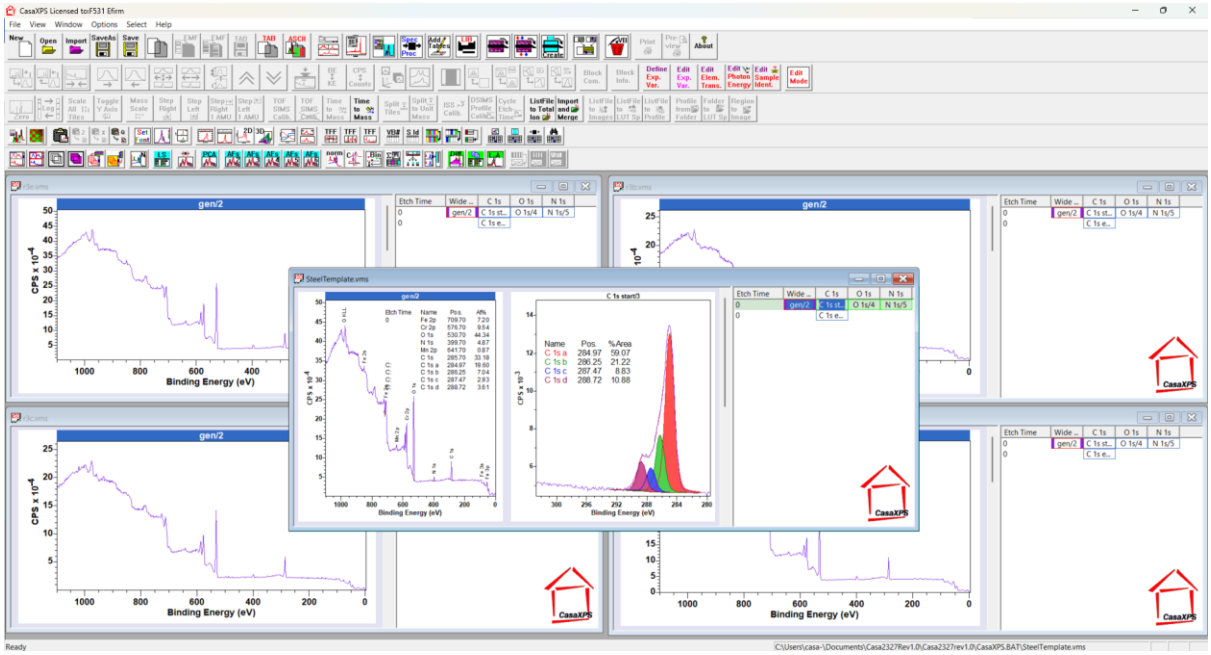

Figure 1. An example of a template VAMAS file prepared with data treatment together with four VAMAS files containing similarly formatted data to the template file. Document-View Model architecture of CasaXPS allows multiple VAMAS files to be open simultaneously. Moreover, data treatments performed on one VAMAS file can be transferred to other VAMAS files. These results may be reported in tabulated format suitable for spreadsheet programs or graphical display of data visualised in CasaXPS exported as enhanced meta file (vector drawn) output that can be inserted into Word.

Introduction

The concept of workflow is germane to users of XPS with routine tasks that are time consuming and repetitive. The objective for enhanced workflow features in CasaXPS is to make such tasks quick and easy to execute. The architecture of CasaXPS (Figure 1) is designed to enhance workflow as well as to support the scientific interrogation of data. The ISO 14976 (VAMAS) format provides spectroscopic data with experimental context, which combined with the options available to manage VAMAS files within CasaXPS facilitate the processing and reporting of results for samples analysed by XPS.

Modern X-ray photoelectron spectrometers are capable of generating data sets of considerable size. Whether data sets contain many or few spectra, it is often the case that a set of quantification regions used to compute elemental quantification or peak models

designed to extract chemical state information constructed for the analysis of one sample are appropriate for similar samples. Moreover, the development of a peak model for a particular material is best done by correlating common chemical bonds between other elements and making use of multiple measurements from similar samples. Research into materials for which XPS provides insights rather than absolute answers needs the ability to test peak models by fitting to multiple spectra all of which are expected to reflect the chemistry of interest. Actions of this type are performed in CasaXPS by propagating data treatment between spectra manually. However, there are occasions where the sample chemistry is known and the objective is to verify that a batch of samples, all of which are, in principle, identical within some tolerance such that it is possible to define all the necessary data treatments and suitable presentation of results to perform the analysis and reporting for these samples. For batches of samples, all of which are measured in an identical way, resulting in identical format for the VAMAS files, an automated method becomes the best way to process large numbers of spectra without the risk of human error preventing a fair comparison of sample composition by XPS.

Overview for two Alternative Approaches to Data Analysis,

1) The Manual Approach: Propagation of Data Treatment between Files Open in CasaXPS and
2) The Automated Approach: Batch Processing of Folders containing yet-to-be-Opened Data files

Propagation Overview

VAMAS (ISO 14976) files opened in CasaXPS make use of the multiple-document view-model for software development. Within the document-view software architecture of CasaXPS, each VAMAS file opened in CasaXPS is added to a list of documents that are linked during a session, which permits the transfer of data treatment from one VAMAS file to some or all VAMAS files opened in CasaXPS. Moreover, each VAMAS file within the list of open documents is viewed through windows that are managed by the CasaXPS main window. Selections of VAMAS blocks within VAMAS files facilitates the transfer of specific data treatments from one type of data to similar data in different VAMAS files. Therefore, the multiple document view model design is the basis upon which the propagation options in CasaXPS are made possible. Indeed, propagation of data treatment (quantification regions, fitting of peak models to spectra, processing of spectra and annotation of spectra) from one or more VAMAS blocks to a set of VAMAS blocks within the same VAMAS file or equivalent VAMAS blocks in any open VAMAS file is the preferred method to explore the nature of data in CasaXPS.

Batch Processing Overview

The design of the user interface in CasaXPS is primarily concerned with scenarios where data require investigation. That is, elemental and chemical state for elements within a sample are of primary concern. Propagation of data treatment is an essential part of examining spectra with these motivations, however, there is a different scenario where the data treatment for samples of similar composition is well known. While the power to transfer data treatment via the propagation features of CasaXPS is capable of rapidly analysing data measured from multiple samples, CasaXPS also includes a method that permits data treatment prepared in a template VAMAS file to be applied to many VAMAS files yet to be opened in CasaXPS. If desired, the application of the template file data treatments and the existence of a tile format file corresponding to the template VAMAS file results in the construction of vector drawn graphical files saved to disk that contain each page of display-tiles that appear in CasaXPS. Following the data treatment performed on each data file within the selected folder, a consolidated quantification report for the set of data files is also made available. That is, batch processing (available from the File menu of CasaXPS) allows a specific set of data treatments to be applied to an entire folder containing data files that have been acquired identically to the template file containing the data treatments used to prepare the yet to be processed files. The VAMAS files shown in Figure 1 is an example of four VAMAS files with identical format to a template VAMAS file containing the desired data treatment for each of these four unprocessed VAMAS files. These files in Figure 1 illustrate the nature of data formatted to be suitable for batch processing in CasaXPS.

Designing Acquisition of Spectra to Support the use of Batch Processing

At the core of batch processing is the template VAMAS file used to define all the data treatments required for a particular type of sample. Within the template file is a set of VAMAS blocks. The order of these VAMAS blocks and the strings used to label these VAMAS blocks are important for batch processing. When designing an experiment for samples for which batch processing is desired, it is important to use the exact same experiment program used to construct the template VAMAS file to acquire data from the samples requiring processing. Even when data are processed manually making use of the propagation features in CasaXPS, consistency in naming in VAMAS blocks relating to spectra (block identifier string, element/transition strings etc) and order of VAMAS blocks is helpful. However, in the case of batch processing, consistency between the template VAMAS file and the target files is essential.

Video Narrative for Batch Processing of VAMAS files

The following is a narrative for the accompanying video in which a comparison between batch processing and manually processing VAMAS files both achieve the same outcome. The subject for the video is a set of VAMAS files containing spectra measured from a set of steel

samples. The target of the video is to demonstrate the steps that transfer data treatment (energy calibration, quantification regions and chemical state analysis by fitting of peak models to spectra) from one VAMAS file (the template file) to a set of VAMAS files. The batch processing approach to completing a task as described is to create a VAMAS file for which all the data treatments are present therein, then identify a folder of data files to which these data treatments are required. After completing the task by means of batch processing, the video proceeds to complete the same task by means of the propagation options that facilitate the transfer of data treatment from a VAMAS file open in CasaXPS to a set of VAMAS files that are also all open in CasaXPS. The video further demonstrates how batch processed VAMAS files are prepared in CasaXPS such that the desired outcomes of the data treatment are exported to vector-drawn graphical files (EMF) suitable for import to Word or other Microsoft products including PowerPoint and Excel.

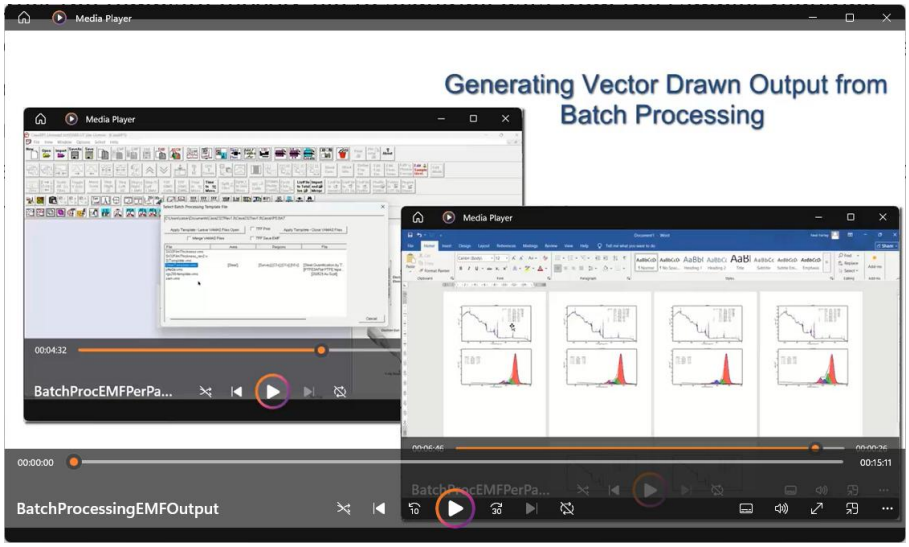

Figure 2. Opening for the video illustrates the vector-drawn graphical files (EMF) created during batch processing entered into Microsoft Word.

Figure 1 illustrates the data treatment and the nature of the VAMAS files that are suitably prepared for either batch processing or manual propagation of data treatment to a set of VAMAS files. The video opens (Figure 2) with an illustration of the intended outcome for the set of spectra shown in Figure 1, namely, each survey spectrum is prepared with quantification regions used to compute percentage atomic concentration displayed over the survey spectrum as an annotation table. Moreover, the survey spectrum includes annotation peak labels for a select group of photoelectron peaks. The data treatment for the VAMAS file also includes a chemical state analysis of the C 1s narrow scan spectrum, which involves the fitting of a peak model to the C 1s spectrum. Furthermore, the template VAMAS file also includes a processing instruction that calibrates the binding energy scale using charge correction and an annotation table are added to the C 1s spectra as shown in Figure 3.

Batch processing is designed to gather quantification results from multiple VAMAS files and create a consolidation report. However, in this example the quantification reports are added

to the display of spectra and the desired output from the actions performed during batch processing is a set of graphical files in a format that can be easily added to a report prepared in PowerPoint or Word. That is, no separately compile text report is required to achieve the goal for the steel samples. Therefore, the template VAMAS file is without a corresponding report specification file (file extension rpt) in the CasaXPS.BAT folder (Figure 4). If the template VAMAS file is accompanied by a report specification file in the CasaXPS.BAT folder the result would be a report in ASCII format tabulating the results of batch processing according to the instructions within the RPT file. However, for this example no RPT specification is available to batch processing. Consequentially, following completion of batch processing a basic report is created, but for the purposes of this video is simply closed in favour of loading the EMF formatted graphical files into Word via a drag-and-drop action.

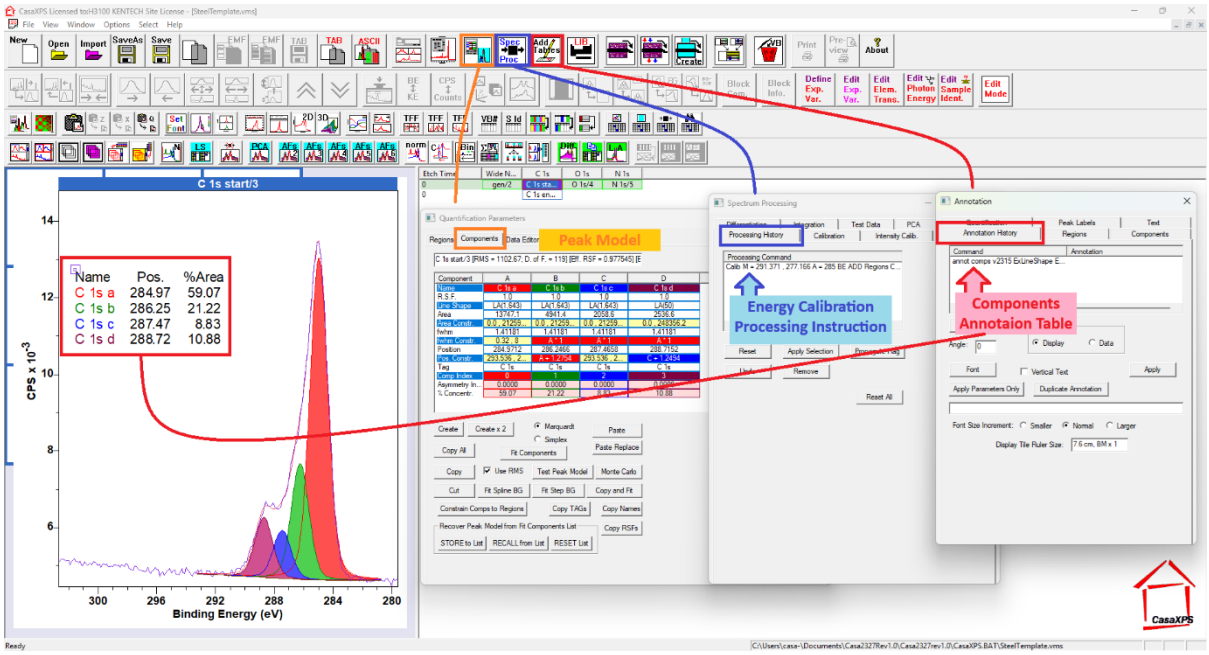

Figure 3. Template file for batch processing. The C 1s spectrum in the template file is prepared with 1) a peak model (both quantification region (not shown) and components listed on the Quantification Parameters dialog window, Components property page), 2) energy calibration (defined using an interval over which the maximum intensity of the C 1s spectrum is aligned with binding energy 285 eV) and 3) an annotation table is added to the display of the C 1s spectrum using the Annotation dialog window.

Since the target for batch processing in this video is to create a display of spectra to include the survey measurement and the C 1s narrow scan spectrum (fitted with a peak model), the precise format for the lefthand-pane of the window in CasaXPS created by batch processing must be specified too. The video illustrates the way a tile format file (TFF) file is placed in the CasaXPS.BAT folder using the same base-name for the TFF file as the template VMS file. Because a TFF file exists in the CasaXPS.BAT folder (Figure 4) with the same base-name as the VMS file selected for batch processing, after each VAMAS file is processed, the TFF file is read and applied to the display state of the processed file. When the EMF files are created,

the display state defined by the TFF file is used to create a new EMF file for each page of tiles that result from loading the TFF file.

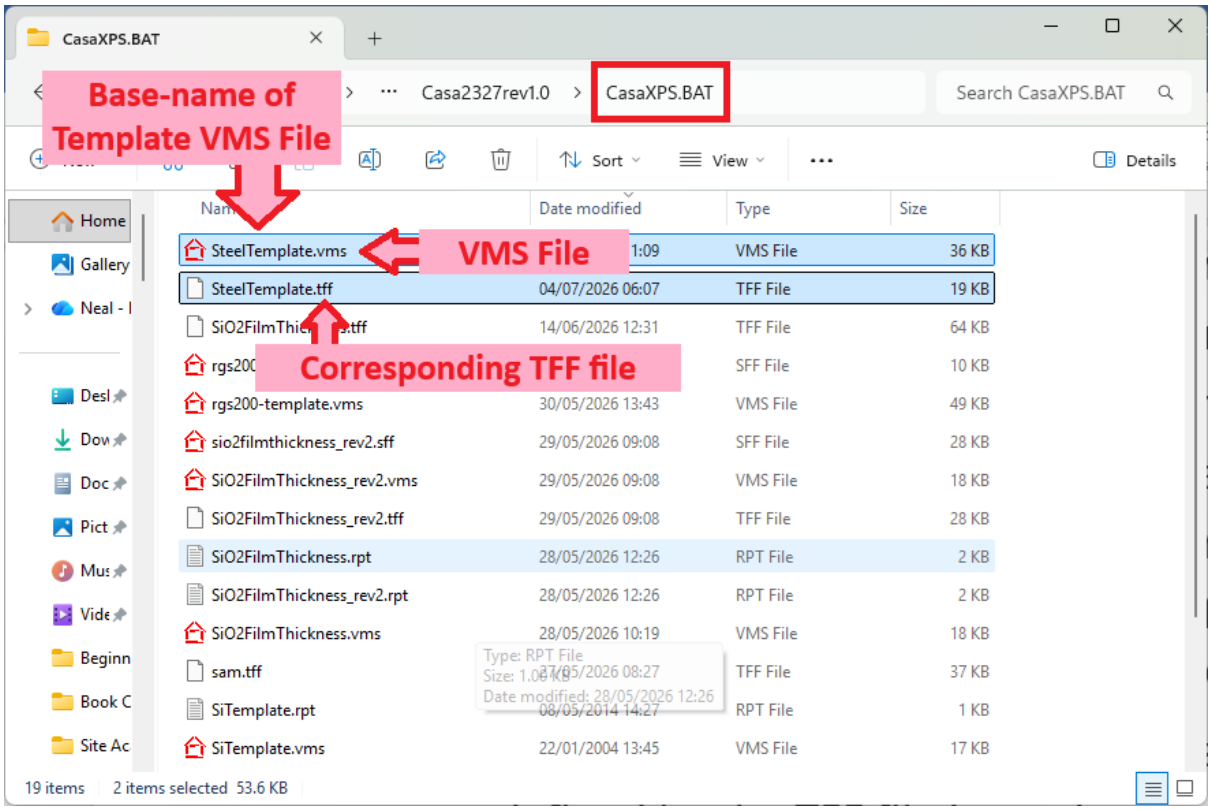

Figure 4. CasaXPS.BAT folder in to which the configuration files used during batch processing are place. The template VAMAS file created for batch processing spectra acquired from steel samples is given the base-name SteelTemplate with filename extension vms. Since, the folder also includes the file SteelTemplate.tff, the result of batch-processing VAMAS files using the data treatment in the VAMAS file SteelTemplate.vms is the lefthand-pane of the CasaXPS window is formatted according to the information within SteelTemplate.tff.

When a VAMAS file is loaded into CasaXPS via the Open or Convert File menu items, the default layout of the lefthand-pane includes one-display-tile per page, where a page corresponds to one or more display tiles visible at any one time in the lefthand-pane. The number of pages that appear in the lefthand-pane is determined by the number of VAMAS blocks that appear in the first row of VAMAS blocks in the righthand-pane. The VAMAS file in Figure 3 contains five VAMAS blocks, four of which are in the first row of VAMAS blocks in the righthand-pane. Therefore, by default, when these VAMAS files are first opened in CasaXPS, the lefthand-pane contains four pages where each page is a single display tile. Since the desire is to create EMF files corresponding to the survey and C 1s spectra, the lefthand-pane must be reformatted to display two pages where the first displays the survey spectrum and the second page displays the C 1s spectrum. Hence the need for a TFF file to reformat the display in preparation for generating the EMF files.

A TFF file is created by preparing the template VAMAS file in the desired layout. Thus, the desired format for the lefthand-pane should be prepared with two pages, the first displaying the survey spectrum and the second page is for the display of the C 1s narrow-scan spectrum. Then, using the File menu of CasaXPS selecting the *Save Tile Format File* menu item allows a TFF file to be created. A dialog window is invoked that allows a TFF file to be saved to disk with a new filename. The TFF file, if not already in the CasaXPS.BAT folder (Figure 4) should be moved to the CasaXPS.BAT folder and the base-name of the TFF file should be renamed to the same name as the base-name of the template VAMAS file. The format of the lefthand-pane is important in determining the number and arrangement of tiles that appear in the EMF files.

There is one more subtilty within the results shown in Figure 2, namely, the selection of VAMAS blocks in the righthand-pane must include the survey spectrum and the C 1s spectrum with the peak model. The need to include the survey and the C 1s spectrum with the peak model in the selection in the righthand-pane is because quantification tables constructed from more than one VAMAS block require the VAMAS Blocks to be on the same row of VAMAS blocks in the righthand-pane. Furthermore, the VAMAS blocks must be selected too. When a VAMAS file is opened via batch processing all the VAMAS blocks are selected by default. While the lefthand-pane format is governed by the definition for the set of VAMAS blocks that are within the TFF file, the selection of VAMAS blocks in the righthand-pane for a VAMAS file processed by batch processing is no longer related to what appears in the lefthand-pane. Moreover, since all the VAMAS blocks in the righthand-pane are selected by batch processing, it is important to ensure the quantification tables, such as the one associated with the survey spectrum, are not compromised by additional quantification items defined on VAMAS blocks other than the survey and C 1s narrow-scan spectra. Specifically, the O 1s and N 1s narrow-scan spectra should not include regions or components that, by virtue of being selected, would be included in the quantification table displayed on the survey spectrum.

While the primary objective for the video is that of batch processing, an additional feature of CasaXPS is also illustrated when preparing the template files for use during batch processing. Namely, the reformatting for the lefthand-pane according to the actions saved within a TFF file. An option on the File menu (Figure 5) is illustrated in the video which makes use of an additional configuration folder (CasaXPS.PTF) into which the template TFF file corresponding to the template VMS file is placed. The sole purpose of using the File menu and the TFF file placed in the CasaXPS.PTF folder is to demonstrate what happens when a TFF file is used during batch processing to create EMF files with specific spectra only. Other than to at some point during the preparation of batch processing configuration files check that the TFF file will recreate the format for the lefthand-pane desired for batch processing of the steel spectra, there is no need to perform these steps (Figure 5) during batch processing itself.

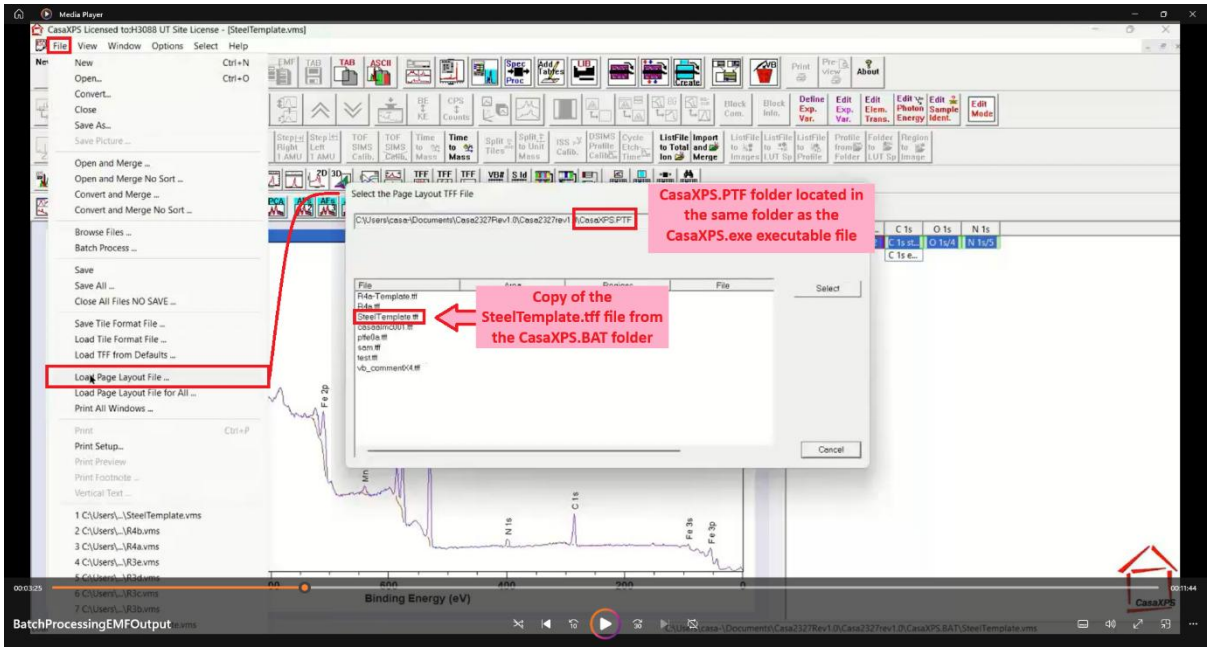

Figure 5. The video demonstrates how a TFF file alters the lefthand-pane of a VAMAS file by applying the TFF file used during the video to batch process the steel samples to the VMS template file shown in Figure 4.

Once all the configuration files are organised in the CasaXPS.BAT folder shown in Figure 4, the steps to perform batch processing that ultimately create the EMF files used in a report are shown in Figure 5. The File menu is used to select the Batch Process menu item that invokes the dialog window shown in Figure 5. The dialog window in Figure 5 displays a list of template-VAMAS-files that corresponds to the set of VAMAS files shown in Figure 4 within the CasaXPS.BAT folder. Once a template VAMAS file is selected and the tick-box labelled *TFF Save EMF* is ticked, the button labelled *Apply Template – Leave VAMAS Files Open*, when pressed, invokes a File dialog window that is used to indicate the folder and the type of file within the folder that represents the target for the batch processing operations. A final dialog window is invoked that allows the batch processing action to be cancelled if necessary. Proceeding with the batch processing of the files within the folder selected via the File dialog window results in the creation of EMF file shown in Figure 7. Note the use of the Convert to VAMAS file dialog window in the video is simply a convenient way to access the functionality of a Windows Explorer type interface that displays files without any filter on the type of files listed. The video illustrates the contents of these EMF files listed in Figure 7 by performing a selection of all EMF files seen in Figure 7, then using a drag-and-drop action of the mouse, the EMF files are entered into a Word document.

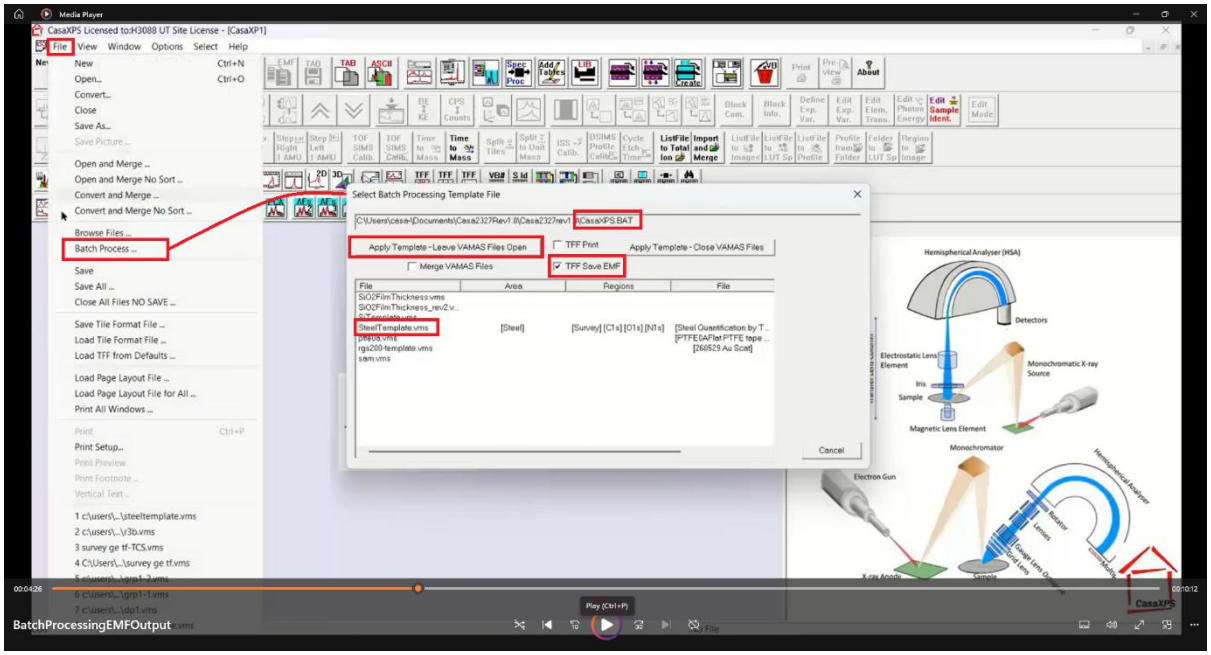

Figure 6. Batch processing of a set of VAMAS files in a folder is initiated from the File menu and selecting the options highlighted on the dialog window boxed-in-red.

The EMF files shown in Figure 7 are created by batch processing from the arrangement of tiles in the lefthand-pane of CasaXPS. Each EMF file corresponds to one page of tiles that can be seen in CasaXPS after the batch processing has concluded. Since the TFF file used to format the lefthand-pane of CasaXPS contains two pages of tiles, and each page of tiles contains one display-tile, the number of EMF files in this example is twice the number of VAMAS files treated. The names for the EMF files reflect the relationship of the EMF file with the originating VAMAS file and the layout for the display of spectra in the lefthand-pane for these VAMAS files when left open in CasaXPS.

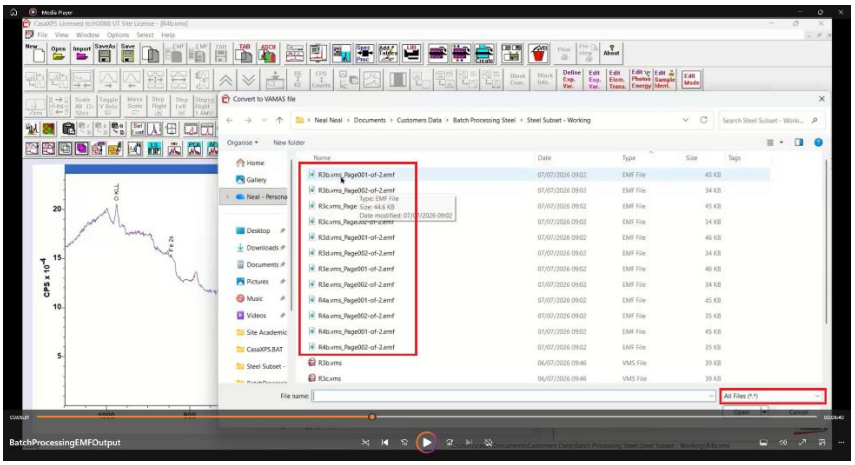

Figure 7. The result of batch processing using the options illustrated in Figure 6 is a set of EMF files written into the folder containing the set of VAMAS files that were the target for batch processing.

EMF files are vector drawn graphical images that can be adjusted in Word, for example, to alter the size of these images. Fonts etc will rescale as the size of the images in Word (shown in Figure 8) are resized.

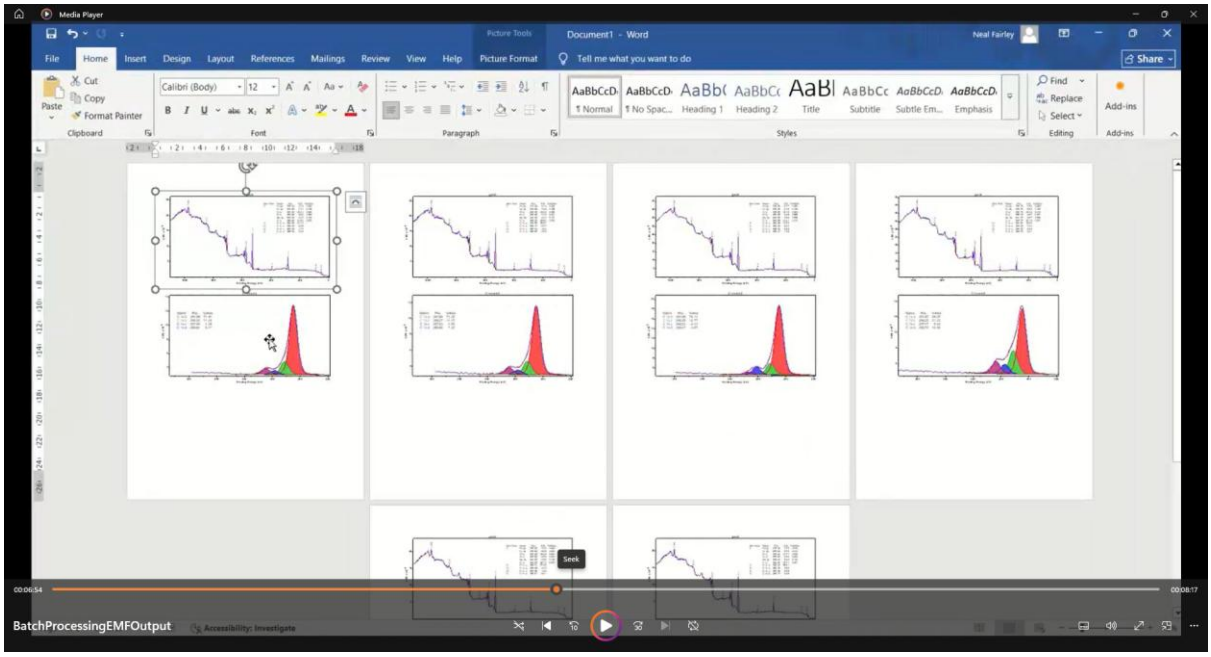

Figure 8. The EMF files created in the folder where the VAMAS files targeted by batch processing are located are dragged and dropped into an open Word document.

The second half of the video repeats the processing of these VAMAS files. The number of VAMAS files used in the video is limited to four VAMAS files for the purposes of the video only. Without the need to illustrate in a video how the selection of VAMAS blocks in many files is achieved, any number of VAMAS files open in CasaXPS could be processed by means of these propagation-operations illustrated in the video. The manner in which VAMAS blocks are selected via the Select menu of CasaXPS is illustrated in other videos. Hence, the narrative of the video does not include further comments about the propagation options in CasaXPS. The remainder of the video simply shows how batch processing helps to perform tasks that could be achieved using the propagate options in CasaXPS, but by using batch processing correctly, the process is less prone to human error.