

CSCD 488

# ICP-OES Text File Parser User Manual

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Version 1.0

## Overview

This document details the use of the ICP-OES Text File Parser. The Parser is a tool developed to parse the data output of Eastern Washington University's ICP-OES machine into a readable Excel file format and perform correlation analysis on the data.



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# 1. How to Use This Manual

## 1.1. Conventions

Significant terms or ideas are **bolded** or, if within an already bolded sentence, the term or idea will be colored **red**.

The Parser requires input from the user to be typed on the keyboard. Sometimes what that input is can vary based on things such as file location and the setup of the user's computer. When this is the case, explanations that detail varying user input will denote what can be varied in angle brackets <>. For example in the sentence "open the <color> door" it is the word "color" that can vary depending on context.

## 1.2. Terms

**Application** or **Parser**: is used to refer to the ICP-OES Text File Parser program.

**Configuration File** or **Config File**: is used to refer to a file that is used by the Parser application and can be edited to represent different parameters that will be used when performing functions.

**Input File**: is used to refer to any file that is to be read, or used as input, by a command.

**Parameter**: refers to part of a command that varies and is inputted by the user.

**Workbook**: refers to a Microsoft Office Excel file that contains one or more worksheets containing related information.

**Worksheet:** refers to a single spreadsheet containing cells organized by rows and columns within an Excel workbook.

## 1.3. Symbols

### **Note**

This indicates supplementary explanations or useful tips about using the Water Analysis Parser.

### **Refer To**

This indicates page(s) relevant to the current location of this section. P. xx is used to refer to pages in this manual.

### **Warning**

This indicates important notices or restrictions.

### **Troubleshooting**

This indicates explanations for errors that may be encountered and how to troubleshoot these errors.

## 2. Quick Start

There are two functions that the Parser will perform. The first of these functions is to generate a formatted Excel spreadsheet from the text file output of the ICP-OES machine. The second of these functions is to perform correlation analysis on the data in that formatted Excel spreadsheet. The Parser is a console application, meaning it waits for commands from the user to be typed into the keyboard. This section describes how to quickly start using these functions.

### 1. After launching the Parser application enter the **parse** command.

The **parse** command takes the form of **parse <file location/name of input file> <file location/name of output file> <method name>** with the method name parameter being optional. See figure 1.



*Figure 1: shows an example of a valid parse command using an input file at C:\Users\Username\Documents\Data.txt and generating an output file at C:\Users\Username\Documents\Formatted.xlsx*

For an in-depth explanation of the parse command see P. 06.

### 2. The application will display success, warning, and/or error messages for the parse command and then await input for another command.

**3. Using the Excel file that was just generated, or using a previously generated file, enter the **analyze** command.**

The **analyze** command takes the form of **analyze <file location/name of input file> <R<sup>2</sup> threshold>** with the R<sup>2</sup> threshold parameter being optional and defaulting to 0.7. See figure 2.



*Figure 2: shows an example of a valid analyze command using an input file at C:\Users\Username\Documents\Formatted.xlsx with an R<sup>2</sup> threshold value of 0.85.*

For an in-depth explanation of the analyze command see P. 19.

**4. The application will display success, warning, or error messages for the analyze command and then await input for another command. At this point, more commands may be entered or enter **exit** to exit the application.**

## 3. Parsing ICP-OES Output Text Files

The major function of the ICP-OES Text File Parser is to take the text file generated by the ICP-OES machine with the measured analyte data and convert, or **parse**, it into a more readable spreadsheet format. Beyond this conversion the Parser also applies quality assurance/quality control color coding to the data and generates a calibration curve. This section explains in detail how to use the **parse** command as well as what the color coding of the parsed data represents.

### 3.1 Using the **Parse** command

The **parse** command reads from an un-altered text file generated by the ICP-OES and writes the data to a new Excel file. The following are step by step instructions on how to use the **parse** command.

It is a good idea to read this entire section prior to generating a text file to be parsed as some of the steps have suggestions and requirements for things such as naming samples of certain types or editing configuration files.

#### **1. Locate the ICP-OES text file that is to be parsed and ensure that it is valid.**

A valid file is one that has not been edited and has a **[Sample Header]**, **[Results]**, and an **[Internal Standards]** section for each sample that was analyzed and each of these sections is separated by a blank line. See figure 3 for an example of a valid file.



*Figure 3: shows an example of a sample in a valid text file that has been created by an ICP-OES machine with spaces between each section and before the [Sample Header] section and after the [Internal Standards] section.*



**2. Check that the **CheckStandards.xlsx** configuration file has a **worksheet** for the **method** that was used when the ICP-OES generated the text file.**

The worksheet corresponding to the method used has the known concentrations for Calibration Standard, Continuing Calibration Verification, and Check Standard samples. The worksheet will be used for calculations, generating calibration curves, and telling the application what elements were tested for. If a worksheet does not exist for the method that was used one will have to be created.

For more information on the use of the configuration file or instructions on how to add a method to the configuration file see see P. 24.

**3. Check that the **Method** being used in the **CheckStandards.xlsx** configuration file has a **Calibration Standards** section.**

If a **Calibration Standards** section does not exist one will need to be added. See figure 4 for an example of a Calibration Standards section.

For an in depth instruction of adding or editing sections in the configuration file see P. 24 or P. 34 respectively.

**4. Verify that the Calibration Standards section has calibration standard concentrations for samples that correspond to the Calibration Blank and Calibration Standards that were measured when the ICP-OES text file was generated.**

If there is not a calibration standard with known concentrations for every calibration standard or blank that was measured one will need to be entered into the configuration file.



*Figure 4: shows an example of the calibration standards section for calibration sample measurements that had a calibration blank and concentrations of 1:5000, 1:1000, 1:500, 1:100, 1:50, and 1:25.*

The Calibration Standards need to be **listed in the order they were measured** in and each must **correspond** to a **measured** Calibration Standard in order for the calibration curve to be generated correctly.

If the calibration standards were not listed in the order they were measured when the calibration curves were generated the rows can be moved to the correct places within Excel and Excel will correct the charts.

Any element that was not measured for or does not have a known concentration for a calibration standard concentration must have a **zero** in its cell (for example, in figure 3, if Al3082 did not have known concentrations that entire column should have zero's in its cells).

For clarity, it is helpful if the calibration standards that are measured are named the same or similar to the calibration standards in the CheckStandards.xlsx config file.

**5. Check that the Method being used in the CheckStandards.xlsx configuration file has a Continuing Calibration Verification (CCV) section.**

If the **Continuing Calibration Verification (CCV)** section does not exist one will need to be added. See figure 5 for an example of a CCV section.

For an in depth instruction of adding or editing sections in the configuration file see P. 24 or P. 35 respectively.

**6. Verify that the Continuing Calibration Verification (CCV) section has known concentrations for a CCV sample that corresponds to the CCV sample that was measured when the ICP-OES text file was generated.**

If the CCV sample with known concentrations does not correspond to the CCV sample that was measured it will need to be replaced with one that does.

If a CCV sample with known concentrations does not exist one will need to be added that corresponds with the CCV sample that was measured.



*Figure 5: shows an example of of the Continuing Calibration Verification (CCV) section for a CCV sample measurement of 1:100 concentration.*

Any element that was not measured for or does not have a known concentration for a CCV must have a **zero** in its cell (for example, in figure 5 if the third concentration was not known a zero would need to be in the place of 0.2).

CCVs that are in the CCV section but were not measured for can be left in the configuration file and will be ignored.

**7. Check that the Method being used in the CheckStandards.xlsx configuration file has a Check Standards section.**

If a **Check Standards** section does not exist one will need to be added. See figure 6 for an example of a Check Standards section.

For an in depth instruction of adding or editing sections in the configuration file see P. 24 or P. 35 respectively.

**8. Verify that the Check Standards section has known concentrations for every Certified Value sample that was measured when generating the ICP-OES text file.**

If a Check Standard sample with known concentrations does not exist for a certified value sample that was measured one will need to be added.



Figure 6: shows an example of the Check Standards section for certified value measurements of samples that correspond to Soil B 1:100, TMDW, and TMDW 1:10.

Certified Value samples will **need** to be **named to match** the corresponding Check Standard in the CheckStandards.xlsx config file.

Check Standards that are in the Check Standard section but were not measured for can be left in the configuration file and will be ignored.

**9. Close the CheckStandards.xlsx configuration file, the input text file that is to be parsed (if it is open) and the Output Excel file (if it already exists and if it is open).**

If the application gives an **error** message that reads "**The process cannot access the file <file name> because it is being used by another process.**" ensure that any file that is being used by the Parser is not open in another application such as Excel or notepad. If they are open, close them and attempt the same command again.

## 10. Launch the ICP-OES Text File Parser application and enter the **parse** command.

In order for the Parser to perform the parse function it will need to be told that the **parse command** is being used followed by the **location and name** of the file to be **parsed**, the **location and name** of the output spreadsheet that is to be **generated**, and optionally the name of the **method** that was used when the input text file was generated. If no method name is entered it will default to the **ICP-SS** method.

When the application is first launched a startup message will be displayed followed by a prompt to enter a command. Using the keyboard, type "**parse <location of input text file\input text file name> <desired location of output Excel file\desired output file name> <method name>**" without the quotes and press enter. Success, warning, and/or error messages will be displayed followed by a prompt to enter another command. At this point more commands can be entered or type "**exit**" and press enter to close the application. See figure 7 for an example of what this step might look like.



*Figure 7: shows an example of using the parse command to parse the file at C:\Users\Username\Documents named Input.txt into the output Excel file named Output.xlsx at C:\Users\Username\Documents.*

If the location of an input or output file contains a space or if the input file, output file, or method names have spaces the location and name will need to be surrounded by double quotes. For example, in figure 7 if the input file with a space in its name was "Lake Samples.txt" one would need to enter the command **parse "C:\Users\Username\Documents\Lake Samples.txt" C:\Users\Username\Documents\Output.xlsx** instead.

If the **error** message "**Error: Parser found zero generic samples. Could not generate formatted Excel sheet.**" Is encountered check that the input text file is properly formatted and has samples of the type "UNK" that correspond to the generic samples that were measured by the ICP-OES. Attempt the command again

If the **warning** message "**Warning: Encountered a Certified Value sample whose check standards were not present in the CheckStandards.xlsx config file. Sample data will be missing from output file.**" is encountered check that the configuration file and the method worksheet being used has a **Check Standard** that corresponds to the certified value that was measured in the file. If one exists make sure both names are the same. If one does not exist add it to the **Check Standards** section. Attempt the command again.



If the **error** message "**Error: Could not write Calibration standards to Excel Worksheet. Reason: ...**" or "**Error: Calibration curves could not be generated. Reason: ...**" is encountered ensure that the **Calibration Standards** section in the configuration file is formatted correctly with zeros in cells for elements with no known concentrations and columns for every element that was measured in the calibration standard samples. Attempt the command again.

It is not necessary that file extensions (such as .txt or .xlsx) need to be added to the names of input and output files. For example, in figure 7 one could enter the command **parse C:\Users\Username\Documents\Input C:\Users\Username\Documents\Output** instead.

In order to remove the need to enter the location in each command place input files in the same location as the application. For example, if, in figure 7, the input file was in the same location as the application and an output file was to be generated in the same location one would enter the command **parse Input.txt Output.xlsx** instead.

## 3.2 Understanding Quality Control/Assurance Color Coding

The **parse** command applies color coding to analyte data to represent different failures or successes.

### 3.2.1. Percent Recovery

Percent recovery is a measure of accuracy.

- Any percent recovery calculation that is less than 90% or greater than 110% is colored **red**.

### 3.2.2. Analyte Data Compared to Blank LOD, LOQ, and Percent Recovery

Comparing analyte measurements to Limit of Detection (LOD), Limit of Quantification (LOQ), and percent recovery can indicate measurements that are not trustworthy and ones that are.

- If an analyte concentration is less than the corresponding LOD it is colored **red**.
- If an analyte concentration is less than the corresponding LOQ but greater than the corresponding LOD it is colored **orange**.
- If an analyte concentration is similar to the corresponding concentration of a check standard that has a poor percent recovery it is colored **blue**.
- If the analyte concentration for a procedural blank is greater than 5% of any general corresponding analyte concentration that analyte concentration is highlighted in **red**.
- Any analyte concentration is higher than the highest corresponding calibration concentration that analyte concentration is colored **purple**.
- All other analyte concentrations are colored **green** to indicate these data are good to use.

These QC/QA formatting rules are adapted from the document **Standard Operating Procedure for EWU Geochemistry Lab: Quality Control and Quality Assurance**. Review this document for more information on using ICP-OES data for research papers, reports, etc.

## 4. Performing Correlation Analysis on Analyte Data

The second function of the ICP-OES Text File Parser is to perform correlation analysis on analyte data by calculating  $R^2$  values for analyte pairs, generating a correlation matrix with those values, and finally generating charts for analyte pairs with high  $R^2$  values. This section will explain in detail how to use this functionality with the **analyze** command.

### 4.1 Using the Analyze Command

The **analyze** command reads data from Excel spreadsheets that were generated by the **parse** command (but may have been altered manually) and adds a worksheet to this file containing correlation matrices and analyte pair graphs. Follow these instructions step-by-step to ensure no errors are encountered.

1. **Locate the Excel spreadsheet (.xlsx) file that contains the analyte data that is to be analyzed and ensure that it is valid.**

A valid file is one that has a header that reads "**Samples**" somewhere in the first column followed by any number of individual sample group headers with at least **more than one sample** in them. A valid file also requires that the **element names** are listed starting in cell **C5** and continuing in that row. See figure 8 and 9 for examples of a valid Excel file.



*Figure 8: shows an example of how the element names should be formatted in an Excel spreadsheet that can be analyzed.*



*Figure 9: shows an example of the "Samples" header and two sample groups in an Excel spreadsheet that can be analyzed.*

Sample groups must have a blank row separating the last sample in the group and a new sample group header. See figure 9 for an example of how this should look.

An input file can be edited to include other sample groups from different parsed files. They just need to be added below the "Samples" header and separated from other sample groups by a blank row.

## 2. Close the Excel spreadsheet (.xlsx) file (if it is open).

If the application gives an **error** message that reads “**The process cannot access the file <file name> because it is being used by another process.**” ensure that the Excel file to be analyzed is not open in another application such as Excel. If it is open, close it and attempt the same command again.

## 3. Launch the ICP-OES Text File Parser application and enter the analyze command.

In order for the application to perform the analyze function it will need to be told that the **analyze command** is being used followed by the **location and name** of the file containing the data to be analyzed and, optionally, a **minimum threshold** for  $R^2$  value. If no  $R^2$  threshold value is entered it will default to **0.7**.

When the application is first launched a startup message will be seen followed by a prompt to enter a command. Using the keyboard, type “**parse <location of input Excel file>\input Excel file name> < $R^2$  threshold>**” without the quotes and press enter. Success, warning, and/or error messages will be displayed followed by a prompt to enter another command. At this point more commands can be entered or “**exit**” can be typed and enter pressed to exit the application. See figure 11 for an example of what this step might look like.



Figure 11: shows an example of using the *analyze* command to analyze data in the Excel file at C:\Users\Username\Documents named *Analyze.xlsx* with an  $R^2$  threshold of 0.9.

If the location of the file to be analyzed or the file name itself contains spaces the location and name will need to be surrounded by quotes. For example, in figure 11, if the file to be analyzed was named "Lake Samples.txt" one would need to enter the command **analyze** **"C:\Users\Username\Documents\Lake Samples.xlsx"** instead.

If the **warning** message "**Warning: Standard deviation for <element name> is zero. Some  $R^2$  values may be missing.**" is encountered this may mean that the element may not have been measured for in the sample group being analyzed. If the element was measured for in the sample group being analyzed check that the data in those cells are numeric and different enough to have a non-zero standard deviation.

If the **error** message “**Error: To calculate standard deviation the length of a set must be greater than 0. Problem with <element name>.**” or “**Error: To calculate covariance the length of both sets must be equal and greater than 0. Problem with <element name> and <element name>.**” is encountered check that the sample group being analyzed has data for the element(s) named. If not analysis cannot be run on this sample group.

It is not necessary for file extensions (.xlsx) to be added to the name of input file. For example, in figure 11 one could enter the command **parse C:\Users\Username\Documents\Analyze** instead.

In order to remove the need to enter the file location in each command place input files in the same location as the application. For example, if, in figure 11, the file to be analyzed was in the same location as the application one would enter the command **analyze Analyze.xlsx 0.9** instead.



## 5. Configuration File and Methods

In order to perform all of the functionality of the **parse** command the ICP-OES Text File Parser relies on a **Configuration File**, named **CheckStandards.xlsx**, that provides data not present in the ICP-OES text files for the known concentrations of certain sample groups. The configuration file is an **Excel Workbook** (.xlsx) that contains one or more **worksheets** representing different **methods** that were used by the ICP-OES to generate text files with analyte measurements. Each method has a section for known concentration of **Calibration Standards**, **Continuing Calibration Verification (CCV)**, and **Check Standards**. This section will discuss how to add method worksheets to the configuration file and procedures for editing existing worksheets.

If an **error** message is encountered when running the **parse** command that states "**Error: The CheckStandards.xlsx config file does not exist or could not be found and the input file could not be parsed.**" this means that the CheckStandards.xlsx config file is not in the **same location** as the application. To solve this **move** the config file to the same location as the application or **create** a new .xlsx named **CheckStandards** and follow the steps in section **5.1. Adding a Method Worksheet**.

### 5.1. Adding a Method Worksheet

Method worksheets need to be added whenever a method was used by the ICP-OES to measure water samples and that method does not already exist in the **CheckStandards.xlsx** configuration file. By default the application will use the **ICP-SS Method** worksheet unless otherwise told in the **parse** command. The following steps will describe how to create a **new method worksheet**.

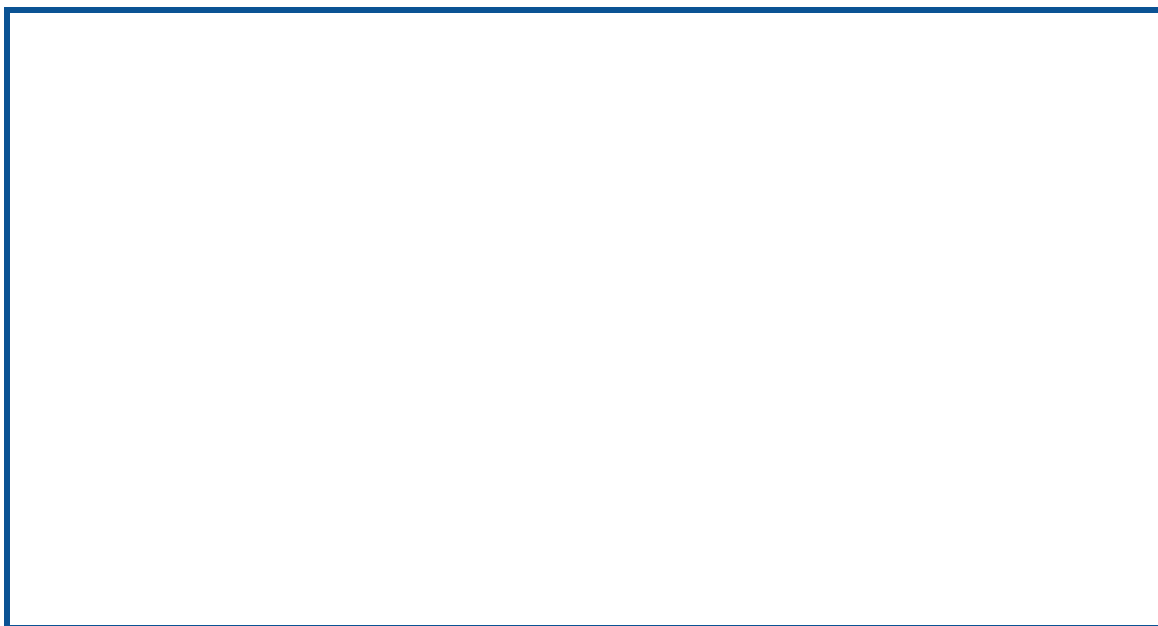


Figure 13: shows an example of what the a worksheet for a method named ICP-SS might look like. *Element Headers:* Note that the element names start at column C row 3 and continue on in the same row with one element per column. *Sample Sections:* Note that in each different sample section sample names are in the first column and the analyte concentrations start in the third column matching up with the element name headers.

**1. Open the *CheckStandards.xlsx* Excel Workbook in Microsoft Office Excel.**

**2. Add a new worksheet.**

Worksheets can be added by locating and selecting the plus symbol in the bottom left of Excel, see figure 12. Alternatively, to add a worksheet, navigate to Home -> Insert -> Insert Sheet.



Figure 12: shows the location of the plus symbol used to add new worksheets. In this image it is to the right of the ICP-SS Method Tab.

### 3. In cell **A1** enter the name of the **new method**.

This will be the method name that is entered when using the **parse** command for a text file that was generated using this method. Make sure it is **unique** from any other methods in the config file.

If an **error** message is displayed when running the **parse** command that states "**Error: Could not find a configuration sheet that matches the method: <method name>**" double check each method name in cell A1 and ensure that it matches the method name entered into the parse command. Spelling, symbols, and capitalization all must **match**.

### 4. In cell **C3** and continuing for each column in the third row, begin entering the **element names** in **alphabetical order** for each element that is measured for in this method.

This serves as the header row for the table of element concentrations indicating what element concentrations correspond to. For readability it is recommended that these cells are **bolded**. See figure 13 above for an example of what this header rows should look like.

If element names are not entered in alphabetical order some calculations and quality control/assurance formatting done when running the **Parse** command will be incorrect.

**5. In cell C4 and continuing for each element column, begin entering the units the known concentrations are in.**

This serves as another header row for the table of element concentrations indicating the units of the concentrations. For readability it is recommended that these cells are **bolded**. See figure 13 above for an example of what this header row should look like.

**6. In the first column of the row below the row containing the units create the Calibration Standards section header by typing "Calibration Standards" (sans quotes) and bolding it.**

This serves to indicate where the known concentrations for Calibration Standards samples start. For readability it is recommended that this cell is **bolded**. See figure 13 above for an example of a Calibration Standards section.

**7. In the first column of the row below the row containing the Calibration Standards header begin entering calibration standard sample names that are used in the method and element concentrations for that sample in the corresponding element column.**

Any samples that do not have a concentration for an element but that element is measured for by the ICP-OES using this method must be inputted as a **zero**.

- 8. Skip a row below the last Calibration Standard sample and in the **first column** of the next row create the Continuing Calibration Verification (CCV) section header by typing "**Continuing Calibration Verification (CCV)**" (sans quotes) and **bolding** it.**

This serves to indicate where the known concentrations for CCV samples start. For readability it is recommended that this cell is **bolded**. See figure 13 above for an example of a CCV section.

- 9. In the **first column** of the row below the row containing the CCV header begin entering CCV **sample names** that are used in the method and **element concentrations** for that sample in the corresponding element column.**

Any samples that do not have a concentration for an element but that element is measured for by the ICP-OES using this method must be inputted as a **zero**.

- 10. Skip a row below the last CCV sample and in the **first column** of the next row create the Check Standards section header by typing "**Check Standards**" (sans quotes) and **bolding** it.**

This serves to indicate where the known concentrations for Check Standard samples start. For readability it is recommended that this cell is **bolded**. See figure 13 above for an example of a Check Standards section.

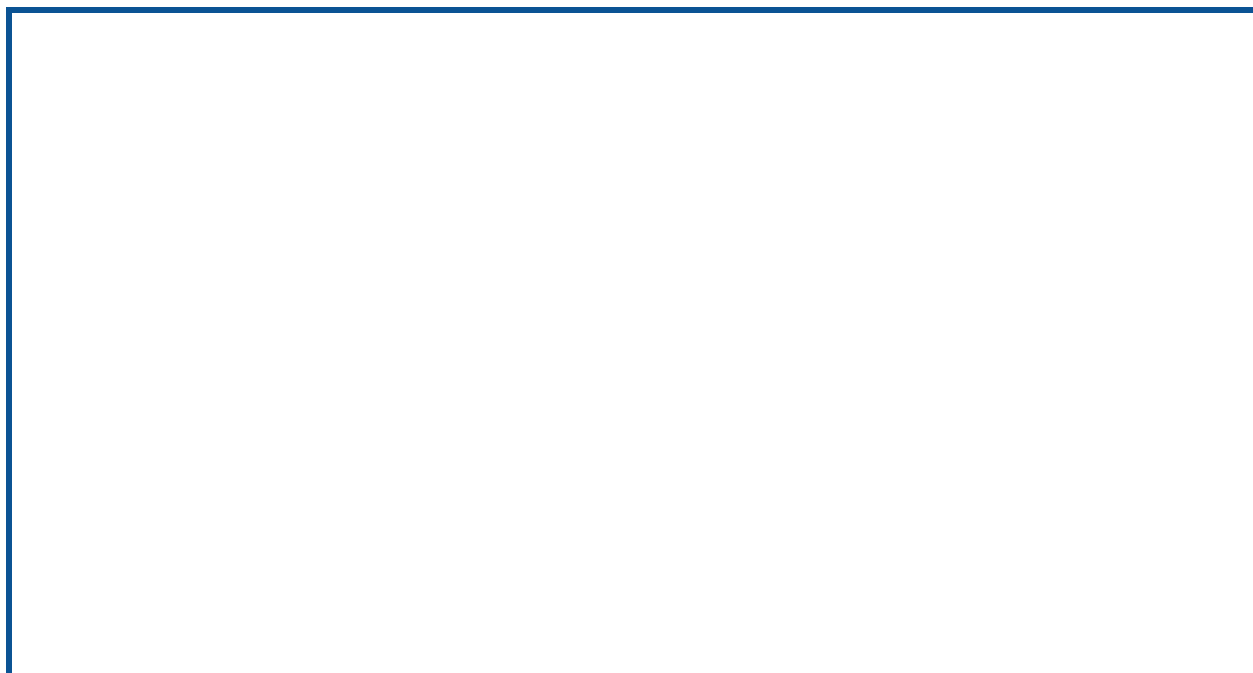
- 11. In the first column of the row below the row containing the Check Standards header begin entering Check Standard samples names that are used in the method and element concentrations for that sample in the corresponding element column.**

Any samples that do not have a concentration for an element but that element is measured for by the ICP-OES using this method must be inputted as a **zero**.

- 12. Save (ctrl + s) the worksheet and close Excel.**

## 5.2. Editing A Method Worksheet

Methods within the CheckStandards.xlsx configuration file can also be edited, but in order for the Parser application to work, certain features must remain unaltered. The following will list what can be edited and how to make those edits and what must not be changed.



*Figure 14: shows an example of a method in the CheckStandards.xlsx configuration file called ICP-SS which tested water samples for Aluminum, Arsenic, Barium, Calcium, Cadmium, and Chromium. Blue highlighting shows what can be edited safely.*

### 5.2.1. What Can Be Edited

Refer to figure 14 above for an example of a method worksheet in the CheckStandards.xlsx config file.

- **Number of elements.**

Any number of elements can be present within a method as long as the number of elements present on the method worksheet equals the number of elements that will be measured in the check standards samples. The following steps describe how to **add** an **element**.

1. Find an **existing element name** that the new element name comes **before alphabetically**. **Right click** on the column letter of that element and select **"Insert"**.

If element names are not entered in alphabetical order some calculations and quality control/assurance formatting done when running the **Parse** command will be incorrect.

2. In **row 3** of the **new column** enter the **name** of the new element.

For readability, it is recommended that the new element name is **bolded**.

3. In **row 4** of the **new column** enter the **units** for the new elements known concentrations.

For readability, it is recommended that the new element name is **bolded**.

4. For each **existing sample** input the **known concentrations** in the **new column** in the corresponding row.

If a sample does not have a known concentration for the new element a **zero** must be entered in the new column for that sample.



- **Amount of samples in each sample section.**

Any sample section (Calibration Standards, CCV, and Check Standards) can have any number of samples with known concentrations. The following steps describe how to **add a new sample**.

1. In the **sample header section** that the new sample belongs to **right click** on the **row number** of the last sample in the section and select **"Insert"**.

If the sample section the new sample belongs to is the **Calibration Standards section** the sample will need to be **inserted** in the **order that the calibration standard samples are measured** in by the ICP-OES.

2. In the **first column** of the **new row** enter the **samples name**.

If the new sample belongs in the **CCV** or **Check Standards** section the sample name will need to **match** the **corresponding samples name** given to the ICP-OES.

3. Starting in the **third column** enter the **known concentrations** for the sample in each column that corresponds to the element.

If an element in the new sample does not have a known concentration a **zero** will need to be entered in that elements column.

- **Names of samples in each sample section.**

The names of samples can be changed by editing the cell containing the name.

If the sample is in the **CCV** or **Check Standards** section the sample name will need to **match** the **corresponding samples name** given to the ICP-OES.

- **Known concentrations for each element in each sample.**

Known concentrations can be changed to any **numerical value**.

If an element in a sample does not have a known concentration a **zero** will need to be entered in that elements column.

- **Known concentration units.**

Known concentrations units can be changed to any measurement but should be the same for each element.

- **Method name.**

The method name can be changed to anything but remember that in order to use a method worksheet when parsing the method name must be entered.

### 5.2.2. What Cannot Be Edited

- **The configuration file cannot be renamed from CheckStandards.xlsx.**

Renaming the config file will cause the Parser to be unable to perform the **parse** command.

- **The configuration file must always be in the same location as the Parser.exe application.**

Moving the config file will cause the Parser to be unable to perform the **parse** command.

- **A method worksheet with a method name of ICP-SS must always be present in the CheckStandards.xlsx file.**

This is the default method used when a specific method name is not entered in the **parse** command.

- **The method name must be in cell A1.**

When using the **parse** command the method name entered is searched for in this cell in each worksheet in the config file.

- **Element names must start in column C, row 3 and continue in row 3.**

The Parser expects element names to always start in this column and be on this row.

- **Element concentration units must start in column C, row 4 below the element names and continue in row 4.**

The Parser expects element names to always start in this column and be on this row.

- **The number of samples in the Calibration Standards section must equal the number of calibration samples that are measured when using the method.**

An unequal number of samples will cause calibration curves and potentially quality control/assurance formatting to be incorrect.

- **Any element does not have a known concentration must contain a zero.**

Samples without a value for each element will cause the sample to be read incorrectly resulting in errors when running the **parse** command.