



Processing multiple datasets
using Topas.

Introduction

There are several ways of refining multiple datasets using Topas depending on the type of data you have collected.

Advantages:

1. it allows some automation e.g. a sequence of potentially hundreds of datasets can be refined in sequence automatically.
2. You can refine parameters over multiple datasets, reducing the error in the parameter over a larger sample.
3. You can refine other parameters systematically with sequence number over the datasets.

However, “rubbish in = rubbish out”.

Topas is not a black box – make sure you understand what you are refining and the parameters you have chosen.

With any kind of multiple dataset processing it is essential to keep on top of your filenames. If they are a sequence, number them accordingly.

Introduction

This tutorial assumes you are familiar with using Topas in interface mode.

All files necessary can be found in the .zip file which can be downloaded from:

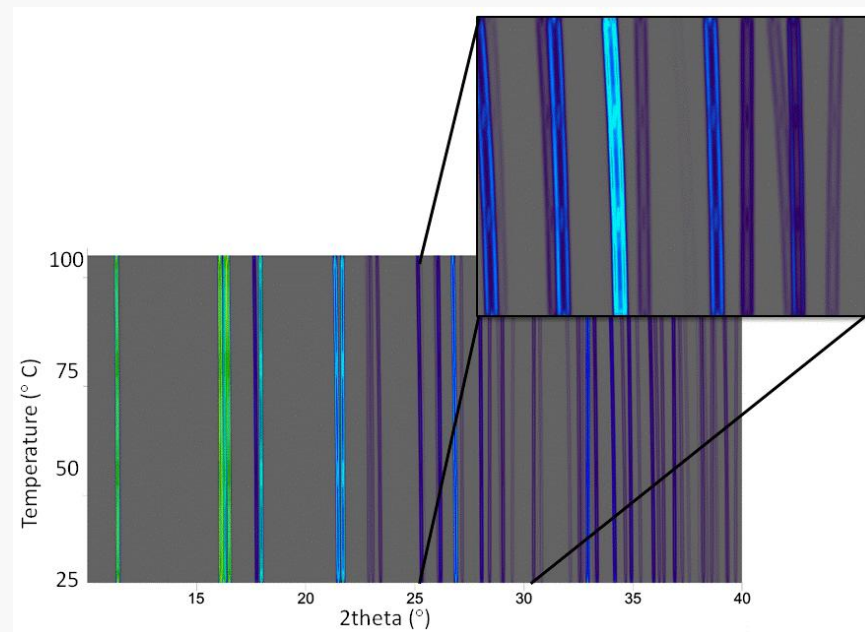
www.synchrotron.org.au

There is a word document in the .zip file with much greater explanation of the tutorials than are included in these slides.

A set of calculated patterns is used here to keep the .inp files as simple as possible for demonstration purposes.

Unit cell variation was produced by applying polynomial expressions to the unit cell.

The files from one example here carry on to the next exercise.



Tutorial Outline: Types of multiple dataset processing

Batch Processing

- Example 1: General batchfiles

- Example 2: Running Topas from a batchfile

- Example 3: Fully automated Topas batchfile

Parametric Refinement

- Example 4: Simple Parametric refinement

Example 1: General Batch files



In this example a series of diffraction patterns have been incorrectly named and the batchfile renames them.

- A batchfile feeds a string of commands to a command line.
- Batchfiles have the extension `.bat`
- This example is designed to be an introduction to using batch files and doesn't involve any Topas refinements.

You will need:

1. `xy` files starting with `"calc_"`
2. `Rename.bat`

These files can be found in the accompanying `.zip` file.

- **Suggestion:** move these files to their own folder named **"Example 1"** so you can keep track of them.

Example 1: “Rename.bat”

- Initially, the filenames are of the form “*calc_temperature*”.
- Open “rename.bat” and you will see that it is just a series of command strings e.g.

```
Rename calc_25 kieserite_25  
Rename calc_30 kieserite_30
```

- The first of these instructs the command line to rename the file “calc_25” with the filename “Kieserite_25”
- The string is then repeated to rename all the available files.

To run the batch file:

Either: double click on rename.bat

or

Type **rename** into a command window opened in the folder where the batch file sits.

Topas and the command line.

- Topas can be run from a command line
- The command line executable is: tc.exe
- It can be found in the main Topas directory

To run Topas from a command line

1. Open a command window and navigate to the Topas directory
2. The command to run Topas is just to type “tc” and follow it with the path to the input file you wish to run.

e.g. `tc C:\Parametric_refinement\kieserite_25.inp`

Thus, by combining Topas with a batch file, refinements can be automatically run from a command line.

Suggestion: Users should be careful to check the outputs from refinements that they can't “see”.

Example 2

A batch of refinements in Topas where you have already made the input files.

You will need:

1. The kieserite example data files with the form: *kieserite_25.xy*
2. The starting .inp: “Kieserite_25.inp”

- The .inp file can be found in the .zip file, example data files can be created by double clicking on the rename.bat file if the user hasn't already completed Example 1.
- **Suggestion:** move these files to their own folder named “**Example 2**” so you can keep track of them.

Example 2

Generate the .inp files.

- A copy of kieserite_25.inp needs to be made for each corresponding .xy file.
- All that needs to be changed within the new input files themselves from the original kieserite_25.inp is the filename on line 5.

Write the batchfile. Include:

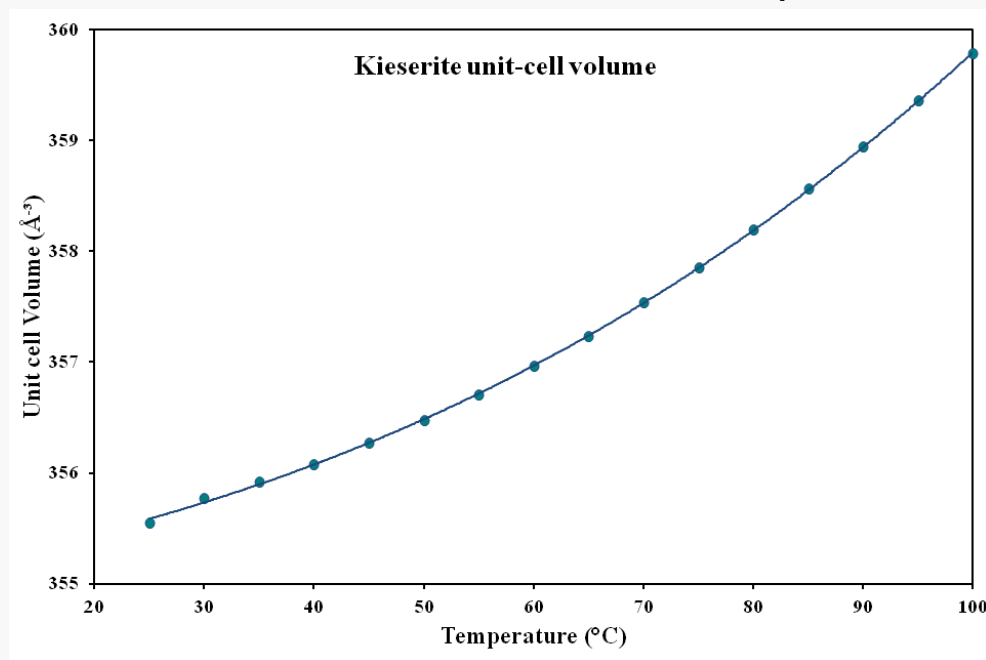
- A line that changes directory where TOPAS is located.
- Lines that instruct Topas to run the .inp files and tells Topas where they are.
- Save the batchfile as “Kieserite_example2.bat”
- **This will produce a batchfile of the form:**

```
cd C:\Topas4-2
tc C:\example_2\kieserite_25.inp
tc C:\example_2\kieserite_30.inp
tc C:\example_2\kieserite_35.inp
```

Run the batch file

Example 2: The results

Plotting the unit cell variation of the kieserite with temperature should give this graph:



The spreadsheet in the .zip file: kieserite.xlsx has the values for the unit cell and cell axes that should be returned from the refinements.

The thermal expansion of the unit cell can then be determined by fitting the data using a polynomial expression (these coefficients are also in the .xlsx).

Example 3:

Running a batch of refinements in Topas where the batchfile automatically generates the input files.

- In this example, we will create a batchfile which runs a sequence of refinements where the output from the previous pattern as the input for the next refinement.

You will need:

1. The kieserite example data files with the form: *kieserite_25.xy*
2. The starting .inp: “Kieserite_25.inp”

- The .inp file can be found in the .zip file, example data files can be created by double clicking on the rename.bat file if the user hasn't already completed Example 1.
- **Suggestion:** move these files to their own folder named “**Example 3**” so you can keep track of them.

Example 3: Alterations to the original .inp file

Open Kieserite_25.inp

The line which instructs Topas which datafile to run must be modified:

It currently reads:

```
xdd Kieserite_25.xy
```

It should be replaced with:

```
#ifndef BATCH  
macro file {"Kieserite_25.xy"}  
#endif  
  
xdd file
```

These lines tell Topas that if it comes across the definition BATCH in it's command line string then it should use the macro "file" which generates the filename for Topas to run (in pink).

Topas will be told what the filename should be in the batchfile.

Example 3: The batchfile

Section A: This section of the batch file cleans the buffer and makes the new input file.

Line 1 deletes any preexisting .inp if the batchfile has been run before.

Line 2 makes the first .inp from the starting inp file the user provides.

```
REM -----
```

```
del C:\Example2and3\Temp.inp
copy C:\Example2and3\kieserite_25.inp
    C:\Example2and3\Temp.inp
```

```
REM -----
```

Section B: Instructs Topas to change directory to the Topas directory (line 1) and run the .inp file (temp.inp) (line 2).

The string beginning "*macro* replaces the filename within the .inp with the appropriate one for the sequence number. In this case the sequence numbers are 25, 30, 35..

```
cd /D      C:\TOPAS4-2\
```

```
TC C: \Example2and3\Temp " macro file { C:
\Example2and3\kieserite_25.xy      } macro seqno {
25 } macro type { KEEP } #define BATCH "
```

Section C: Line 1. Changes back to the directory where the files sit.

Line 2. Deletes previous versions of the .inp file.

Line 3. Creates an output in the form of a .inp file for this refinement from which parameters can be obtained.

Line 4. Creates a .inp file to start the next in the sequence of refinements.

```
cd /D C:\Example2and3\
```

```
del kieserite_25.inp
del Temp.inp
copy Temp.out kieserite_25.inp
rename Temp.out Temp.inp
REM -----
```

Section A need only be included once at the start of the batchfile.

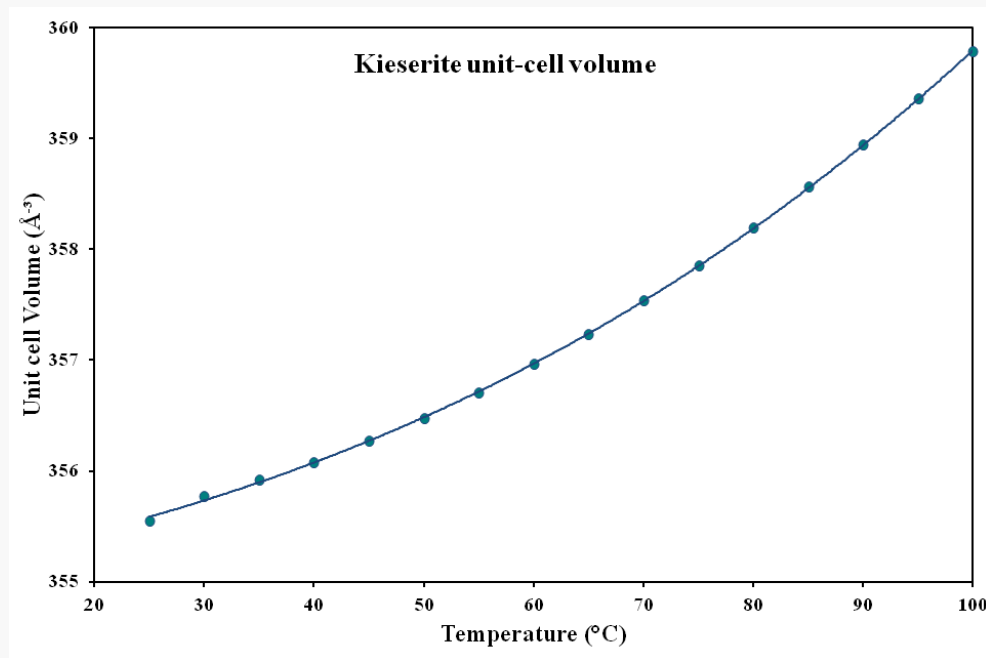
Sections B and C need to be present for each file.

Example3.bat in the included files shows an exemplar, it will run the first 3 datasets.

Fill in for the remaining datasets and then run the batchfile as in Example 1.

Example 3: The results (identical to Example 2)

Plotting the unit cell variation of the kieserite with temperature should give this graph:



The spreadsheet in the .zip file: kieserite.xlsx has the values for the unit cell and cell axes that should be returned from the refinements.

The thermal expansion of the unit cell can then be determined by fitting the data using a polynomial expression (these coefficients are also in the .xlsx).

Example 4:

A “Simple” Parametric refinement.

- Parametric refinements are similar to batchfiles in that they involve the refinement of multiple datafiles.
- However, where they differ is that parameters are tied together over all datasets, rather than being separately refined over a sequence of refinements.
- These parameters are assumed to vary systematically with sequence number through the datasets.
- In this example the unit-cell will be fitted with simple polynomial expressions:

$$\text{Each axis: } a = t_0 + (T \times a_1) + (T^2 \times a_2)$$

$$\text{The beta angle: } \beta = t_0 + (T \times a_1).$$

Advantages:

1. Parameters which are constant over all the datasets, can be refined to a much higher accuracy.
2. Parameters which vary systematically over the datasets, e.g. unit cell parameters on warming, can be fitted automatically as the refinements progress.

Example 4



You will need:

1. The kieserite example files with the form: *kieserite_25.xy*
2. The starting .inp: “Kieserite_para_start.inp”

- The .inp file can be found in the .zip file, example data files can be created by double clicking on the rename.bat file if the user hasn't already completed Example 1.
- The input file kieserite_para_start is setup to run a parametric refinement using the first three of the kieserite datasets.
- The input file has been divided up into sections, the contents of which will now be explained.

Sections I – III: General refinement information



Section I is the goodness of fit data, rwp etc.

Section II is the refinement information such as wavelength, convergence criteria and fit range. It has been constructed as a macro which can be placed into the area assigned to each dataset.

Section III is structural information which remains constant over all the datasets and can be placed into each dataset. These macros help to keep the input files tidy.

Sections IV – VI: Parameter definitions



Section IV defines the datasets to be used in terms of sequence number and these can be turned on or off by commenting the line in or out using a comma at the start of the lines.

Section V gives each sequence number a corresponding value of the parameter which varies throughout the datasets. In this case it is the temperature at each dataset.

Section VI defines the coefficients for the expressions used to fit the lattice parameters. In this case the lattice parameters are to be fitted using simple polynomials, but in practice any analytical expression could be used.

Section VII



Section VII: Information for the refinement of each dataset. It contains the filename, macro keywords as defined in sections II and III and the expressions to fit the lattice parameters as equations.

What to do:

Fill in the information in sections IV – VII for datasets 40 – 100 and then the full range of data will be refined.

To run:

As you would for any launch mode input file, ie select the file as the input file and press play.

Note: The refinements may be slow as Topas requires a fair amount of computing power to refine this many datasets simultaneously.

Example 4: The results

The coefficients returned for the unit cell parameters should be of the order:

a axis

t0	6.888
t1	0.000002
t2	0.000005

b axis

t0	7.6225
t1	0.000005
t2	0.000006

c axis

t0	7.55
t1	-0.000003
t2	-0.000002

beta angle

t0	116.295
t1	0.0002