# Script An introduction

(For Beginners)



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# **1** Introduction

In research/industries, simple electrochemical experiments are carried out multiple times to ensure the quality and reproducibility of a system/product under investigation (i.e., testing of a battery). Using our script program, a simple script can be written, which runs the desired experiments (EIS, potential/current experiments etc) single or multiple times in a predefined order and simultaneously save the measured data in a designated folder. Scripts can also be used to run the experiments when predefined conditions (i.e., current stability, trigger) are met.

The sample scripts from *Section 5* of this manual are also provided in the **c:\thales\script\myscript** folder. The user is welcome to use these scripts as they are or modify them according to his or her requirements. After reading this script manual and working on the sample scripts, the users will be able to write his/her scripts.

This manual will serve as a starting point for users to familiarize themselves with the Zahner script software. For writing the more complex scripts, please read our **Script** and **andiBASIC** manuals. For further assistance contact us at **contact@zahner.de**.

# 2 Starting script program

For starting a script program, turn on your Thales software. In the classic view of Thales software, a "**Script**" icon is provided, click on this icon to open the script sequencer window.

A "Script Sequencer" window contains different buttons, details of which are given below

edit script: to open a script window (ZEDIT USB)

check script: to check for the changes in the script

*link script:* to link the script to the script software

save program: to save the script

new script: to start a new script program



By clicking on the *edit script*, a new window (*ZEDIT USB*) will open. The user can write his or her script in this window.

Once a script is written, then click on "*link script*". Now new buttons will appear on the "Script Sequencer" window which will be used to execute the script.

When any change is made in the script, the *"link script"* has to be clicked so that the software can recognize these changes and implement them in the next measurement.

For two scripts in a ZEDIT USB window (explained below), the second button (with yellow text) will only appear when the cursor hovers over the button.

When a script is run, then the progress of the script can be viewed in the Z-Trace window. Z Trace window can be open via clicking on the small Z on the top left part of the Thales software.

# **3 Writing a script**

# 3.1 Color scheme

In the **ZEDIT USB** window, a script can be written with different kinds of commands, variables, constant and remarks, etc. To easily differentiate between different parts of the script and to make reading the script easy, a color scheme is used. Details of this color scheme are given below

Macro commands	: red + bold (i.e. start/end script, open/save measurement file etc.)
SCRIPT system variables	: black + bold (setting potentiostatic or galvanostatic mode etc.)
andiBASIC commands	: pink (loop functions, condition function - if, goto-, etc.)
Software remarks	: green (comments on script-not processed by the processor)
String constants	: blue (file or variable names, folder paths etc.)
Data	: cyan

If a script is opened via the *edit script* icon then the **Z EDIT USB** window will open. A script can be written, modified, and saved from this format. Only the script opened in the **Z EDIT USB** window will be able to link with the script software.

When a saved script is opened directly from a folder then it will open in the **THALES EDITOR** window. Here one can modify the script and save it. However, linking with the software is not possible. For linking the script, it must be opened in the **Z EDIT USB** window via clicking on the *edit script* button in Zahner script program



## 3.2 Basic structure

For every script, a basic structure is needed. In the **ZEDIT USB** window, the script is written within this basic structure. This basic structure is shown below

```
SCRIPT_PATH$="c:\thales\script\myscript"
SCRIPT1
.
.
```

SCRIPT\_END

First, a path is provided where the script file is saved. We suggest making a "myscript" folder in your script folder in *c:\thales\script*. After providing the path, the script1 command is provided to start the script and script\_end to end the script. All the script code will be written between these two commands.

In a single script file, up to 9 scripts can be written and applied to the system under investigation. The basic structure with 9 scripts is shown below

```
SCRIPT_PATH$="c:\thales\script\myscript" 'folder path for script
SCRIPT1 'start script 1
'script body
SCRIPT_END 'end script 1
SCRIPT_END
SCRIPT_END
SCRIPT3
SCRIPT_END
SCRIPT_END
SCRIPT_END
SCRIPT_END
SCRIPT_END
SCRIPT_END
SCRIPT_END
SCRIPT_END
```

The "c" in folder path i.e., **SCRIPT\_PATH\$="c:\thales\script\myscript**" must always be written small.



Comments in the scripts can be written after an apostrophe ('), this part is not read by the script software. An example of such comments is given above

To properly run a script, few additional buttons are required. To access these buttons, copy the *scr\_logo.icd*, and the *scr\_b1.icd* logo from *c:\Thales\Script* to the folder where the script is saved.

The **myscript** folder provided with this manual contains the sample scripts, required logo-files and rule files. Please save this **myscript** folder in **c:\Thales\Script** for the sample scripts to properly work.

The script is saved in the AMOS textfiles (\*.is\_).

# 3.3 Z-Trace USB window

Z Trace USB window shows us the results of a simple script and the progress of the script during operation. In the example given below, a very simple script is written and the result of this script is shown in the Z Trace USB window.

SCRIPT\_PATH\$="c:\thales\script\myscript"
SCRIPT1 'start script
lprint"test" 'print test
SCRIPT END 'end script

<b>Z</b> t	race USE		<u> </u>
Exit	Clear	Font	
test			^
l			
1			×

**SCRIPT\_PATH**\$ sets the path where the script files (buttons, graphics, etc.) are present.

# 3.4 Turn potentiostat on/off

Here, the potentiostat is turned on and a potential of 1 V is applied. The potential is measured and shown in the **Z** trace USB window. At the end of the script, the potentiostat is turned off.

				EX	it Clear Font	
SCRIPT_PATH\$='	'c:\thales\	script\myscri	pt"	Po	tential=	0.999840285795862
SCRIPT1	'start so	cript				
GETPARAM ′ ge	t current o	onfiguration	of potentios	tat <		
Gal=0				)		
GAL=0	'tu	rn on potenti	ostatic mode	(Gal=0 a	nd GAL=0	)
Pset=1		'set potent	ial to 1 V			
Pot=-1		'turn poten	tiostat ON			
SETUPECW	' ap	ply the settim	ngs above			
POTENTIAL	'me	asure potentia	al			
lprint"Potenti	al=",Pact	'print pote	ntial value			
Pot=0	'tu	rn potentiost	at OFF			
SETUPECW	'ap	ply the setti	ngs above			
SCRIPT_END		'end script	:			

If the potentiostat has to be turned on before loading a rule-file (explained later) then it is crucial to use the **GETPARAM** command in combination with the **SETUPECW** command. Otherwise, ECW hardware may load invalid parameters and exhibit an erroneous behavior.

Once the **GETPARAM** command is used in the script with the **SETUPECW** command then for the rest of the script, a new **GETPARAM** command is not required and only the **SETUPECW** command can be used.

A two-line code is necessary to choose a potentiostatic, galvanostatic, or pseudo-galvanostatic mode.

	GAL=1	GAL=0	GAL=-1
Gal=0	-	Potentiostatic mode	Pseudo- galvanostatic
Gal=-1	Galvanostatic mode		

In the above-provided script, Gal=0 and GAL=0 are used to turn the potentiostat on.

By clicking on commands (i.e. **GETPARAM**) with the right button of the mouse, the **Script** and **andiBASIC** manuals can be open to the page where that respective command is explained. This information is very handy for beginners as they have to check the meaning of different commands frequently.

# 3.5 Choosing different channels

Basic Zennium series potentiostats can be extended with the power potentiostats, electronic loads, and multiplexers. These additional devices are connected via EPC42 cards. To access these devices following script code is used

push1:gosub"im5\*,p",SELDEV\_EXT 'Choose channel 1 of EPC42

Here channel number is written after **Push**. A Zennium series potentiostat can hold 4 EPC42 cards, and each card has 4 channels so to choose different channels, channel number = 1,2,3 ..... 16 are used. In the case of RMUX or PMUX, the first 16 channels are assigned to RMUX or PMUX and the EPC42 channels start from 17 onwards.

To access the main Zennium series potentiostat, use the following script code.

push0:gosub"im5\*,p",SELDEV\_EXT 'Channel 0 is assigned to the main Zennium potentiostat



# 3.6 Loop function

#### 3.6.1 Return-until

The scripts provided in section 3.4 can be easily modified with a simple **repeat** - **until** loop command. This will allow the electrochemical workstation (ECW) to keep measuring the potential until a condition is met. A simple trigger is also recommended to stop the loop prematurely or if the code results in a never-ending loop. In the script below, the potentiostat will keep on measuring the applied potential of 0.1 V every 500 ms until the key "q" is pressed on the keyboard.

```
SCRIPT_PATH$="c:\thales\script\myscript"
```

-				
SCRIPT	1		'stai	rt script
	GETPAR	АМ	'get	current configuration of potentiostat
	Gal=0			
	GAL=0			'turn on potentiostatic mode
	Pset=0	.1	'set	potential to 0.1 V
	Pot=-1			'turn potentiostat ON
	SETUPE	CW	' appl	ly the settings above
		repeat		'start loop
		POTENTIAL		'measure potential
		<pre>lprint"Potential="</pre>	,Pact	'print potential value
		pause 500		'wait 500 milli-seconds (ms)
		get KEY\$		'access keybord
		until KEY\$="q"		'press "q" button on keyboard to stop loop
	Pot=0			'turn potentiostat OFF
	SETUPE	CW	′ appl	ly the settings above
SCRIPT	END		' end	script

#### 3.6.2 For-to [step], next

Besides repeat - until loop, for to (step) - next command is also used for the loop function. In the previous example (repeat - until), the potentiostat will keep on measuring potential until the loop is stopped by pressing "q". With for to (step) - next loop, the potentiostat will measure the potential for predefined number and then will exit the loop.

In this script on the following page, the potential will be measured 100 times, every 500 ms. To stop the loop prematurely a new function *if* - goto is introduced. Here pressing, the "q" will force the script software to go to the **LOOPEND**: code.

During script, **POTENTIAL** or **CURRENT** measurements take around 30 ms hence with the script, it is not possible to measure the potential/current faster than the time interval of 30 ms. Therefore, it is advised that for accurate measurements don't run the loops with a time interval of less than 100ms.



SCRIPT_PATH\$="c:\thales\script\myscr	ipt"
SCRIPT1 'star	rt script
GETPARAM 'get	current configuration of potentiostat
Gal=0	
GAL=0	'turn on potentiostatic mode
Pset=0.1 'set	potential to 0.1 V
Pot=-1	'turn potentiostat ON
SETUPECW 'appl	ly the settings above
for t=1 to 100 step 1	'start loop
POTENTIAL	'measure potential
<pre>lprint"Potential=",Pact</pre>	'print potential value
pause 500	'wait 500 milli-seconds (ms)
get KEY\$	'access keyboard
if KEY\$="q" goto LOOPEN	D: 'press "q" button on keyboard to stop loop
next	'next loop
LOOPEND: :	
Pot=0	'turn potentiostat OFF
SETUPECW 'appl	ly the settings above
SCRIPT_END	

If due to erroneous script, the potentiostat enters a never-ending loop, then the user can press the USB knob (on the front panel of the Zennium series potentiostats) downwards to *nmi*. This will force the potentiostat to stop the ongoing measurement. If you interrupt a measurement loop then pay attention to the potentiostat because depending upon the measurement, the potentiostat will stay on and will not be turned off with nmi. If the potentiostat is ON then the **POT** LED at the front panel of the Zennium series potentiostat will be **orange** and if the potentiostat is off then the LED will be **green**.



## 3.7 Subroutines

The subroutines are a handy tool in script coding which allows the use of a single function multiple times in a script. For example, if in a script the user wants to turn on and/or turn off the potentiostat multiple times between different measurements. Then he or she can create subroutines for turning on or turning off the potentiostat and use those despite witing the whole script. Subroutines are usually written at the end of the script. A gosub command is used for the subroutines. The script provided in the Section 3.6.2 is modified using the subroutines

```
SCRIPT PATH$="c:\thales\script\myscript"
SCRIPT1 'start script
gosubPOT ON: 'go to subroutine 1- potentiostat ON
      for t=1 to 100 step 1 'start loop
      POTENTIAL
                        'measure potential
      lprint"Potential=",Pact 'print potential value
                         'wait 500 milli-seconds (ms)
      pause 500
      get KEY$
                         'access keybord
      if KEY$="q" goto LOOPEND:
                                    'press "q" button on keyboard to stop loop
      next
                               'next loop
     LOOPEND::
gosubPOT OFF:
                          'go to subroutine 2- potentiostat OFF
gotoMENU
                          'go to the main menu of Script Sequencer
      POT ON::
                          'Subroutine 1 - potentiostat ON
      GETPARAM
                          'get current configuration of potentiostat
      Gal=0
      GAL=0
                               'turn on potentiostatic mode
      Pset=0.1
                          'set potential to 0.1 V
      Pot=-1
                               'turn potentiostat ON
      SETUPECW
                          'apply the settings above
                               'return to script
      return
     POT OFF::
                          'Subroutine 1 - potentiostat OFF
      Pot=0
                              'turn potentiostat OFF
                          'apply the settings above
      SETUPECW
                          'return to scriptine 1 - potentiostat ON
      return
SCRIPT END
```

In script make sure not to use **a space**, or a **hyphen** (-) in a string or a variable. Hyphen (-) is used as a mathematical operator (minus).



# **4** Electrochemical measurements

After learning the basics of script coding, the next step is the coding for the standard measurement methods using script software.

- 1. Electrochemical impedance spectroscopy (EIS)
- 2. Cyclic voltammetry (CV)
- 3. Current-voltage curve (IE)
- 4. Polarization curve (POL)

#### 4.1 Rule file

For complex measurements (i.e. EIS), a script that includes all the required parameters have to be written. These parameters include a potentiostatic/galvanostatic mode, voltage amplitude, lower frequency limit, upper-frequency limit, applied bias voltage and step-per-decade for different frequency ranges, etc. Similar is true for other measurement processes, that for each measurement, one has to provide information about each parameter/variable. To simplify this process, a rule-file is used which contains all the parameters, needed for the measurement. This way the user does not have to code for these parameters, making the script code for these measurements very simple. For generating a rule file, a process provided below is followed.



measurement), follow the



click on "control potentiostat"

voltage etc. Click "Esc"

## Clicking "Esc" will bring you back to the 2<sup>nd</sup> window and then click "start recording".

ipedance Spectroscoj	by		ipectrum uns until:	03,27.2
	1000MT 1 1 100	100%	SPECTRUM	100%
	TIVE			CROSS
[impedance] / Ω	phas	e /°	impedance 10.8	/Ω 9
30 -		- 120	phase/ -13.0	)
25 -		- 90	frequency/ 12.85	Hz K
20 -		- 60	voltage /* -0.0	/ 1
15 -			current/) 9.117	'n
10	2400000	- 30		
100m 1 3 10 30	100 1K 3K 10K	100K	STOP	)

4. Measure at least 5 data points and then click "stop"



5. Save measurement as "EIS Rule file" in folder c:\thales\script\myscript



Now, this saved file has all the required parameters saved in it and can be used as a base file (**rule-file**) for the EIS measurement(s) in the script. In script code, a "path-command" to the rule-file is necessary, from where the script program will take the rule file for measurement. For EIS measurement, the following code can be added to the script.

```
MEAS_OPEN_EIS(65,"c:\thales\script\myscript","EIS_Rule_file")'open EIS rule file
MEAS_EIS 'perform EIS
MEAS_SAVE_EIS(65," c:\thales\script\myscript","EIS1") 'save EIS with name EIS1
```

NOTE: "65" indicates that the data location is in the computer drive.

# 4.2 Script – EIS measurement at OCP

The script in this section illustrates the measurement of an EIS spectrum for the system under investigation at the open circuit potential (OCP).

```
SCRIPT_PATH$=,"c:\thales\script\myscript" 'script path
SCRIPT1
                                     'start script
MEAS OPEN EIS(65, "c:\thales\script\myscript", "EIS Rule file")'open EIS rule file
MEAS EIS
                                     'perform EIS at OCP
MEAS SAVE EIS(65," c:\thales\script\myscript","EIS1")'save EIS1 (part1)
SCRIPT END
                                           'end script
Here,
GETPARAM
Gal=0
GAL=0
                                     'turn on potentiostatic mode
Pot=-1
                                          'turn potentiostat ON
SETUPECW
                                     'apply the settings above
```

is not necessary because the potentiostatic/galvanostatic mode and potentiostat turn on/off information is also provided in the saved rule file. Since in the rule file, the EIS is measured with potentiostat turned off (at OCP) hence

Pot=0	'turn potentiostat OFF
SETUPECW	'apply the settings above

is also not necessary. However, if EIS is measured at some bias potential then after the EIS coding, code for turning off the potentiostat is necessary.

In the sample scripts, the **GETPARAM** commands are always provided even if the rule file is opened at the start of the script. This is done as a precaution that upon modifying the scripts, the user does not apply any potential or current at the start of the script without **GETPARAM**.



Similarly, for CV, POL, and IE, a rule file can be saved, and then a script can be written for the before-mentioned measurements. Script code for these measurements is provided below

#### CV:

#### POL:

```
MEAS_OPEN_POL(65,"c:\thales\script\myscript","POL_Rule_file")'open POL rule file
MEAS_POL 'perform POL
MEAS_SAVE_POL(65," c:\thales\script\myscript","POL1") 'save POL with name POL1
```

#### IE:

The script program does not support the POL phase 3 measurement in galvanostatic mode. For such a measurement, please use the Sequencer.

If the user wants to run a POL phase 1 measurement in Galvanostatic mode after an EIS measurement then the set amplitude must be set to zero before POL measurement is run. The example is shown below.

```
MEAS_OPEN_EIS(65,"c:\thales\script\myscript","EIS_Rule_file")'open EIS rule file
MEAS_EIS 'perform EIS at OCP
MEAS_SAVE_EIS(65," c:\thales\script\myscript","EIS1") 'save EIS1 (part1)
GETPARAM
Ampl=0 'set amplitude to zero
SETUPECW 'apply the settings above
MEAS_OPEN_POL(65,"c:\thales\script\myscript","POL_Rule_file")'open POL rule file
MEAS_POL 'perform POL
MEAS_SAVE_POL(65," c:\thales\script\myscript","POL1") 'save POL with name POL1
```



# 4.3 ASCII export

Script program saves the measurements in the special formats (i.e., **\*.ism** format for EIS measurement). If an ASCII export is required then the measured spectrum is opened in SIM and then exported into ASCII format.

```
CLRSIM 'initialize SIM
ANA_OPEN_EIS(65,"c:\thales\script\myscript","EIS1") 'open saved EIS1 file
ANA_XASCII(65,"c:\thales\script\myscript","EIS1") 'save EIS ASCII with name EIS1
```

The script provided in Section 4.2 is extended for the ASCII export

```
SCRIPT_PATH$=,"c:\thales\script\myscript" 'script path
SCRIPT1 'start script
MEAS_OPEN_EIS(65,"c:\thales\script\myscript","EIS_Rule_file")'open EIS rule file
MEAS_EIS 'perform EIS at OCP
MEAS_SAVE_EIS(65," c:\thales\script\myscript","EIS1")'save EIS1 (part1)
CLRSIM 'initialize SIM
ANA_OPEN_EIS(65,"c:\thales\script\myscript","EIS1") 'open EIS1 (saved in part1)
ANA_XASCII(65,"c:\thales\script\myscript","EIS1") 'save EIS ASCII with name EIS1
SCRIPT_END 'end script
```

## NOTE:

The output format of the ASCII data of EIS corresponds to the display format in the Thales SIM program. To change the data of the ASCII export, the standard display format of ism files in SIM must be adapted.

To do this, an EIS spectrum must be loaded in SIM. Then the display format can be set accordingly (refer to <u>SIM manual</u> chapter 3.2). To save these settings as the new standard settings refer to <u>SIM manual</u> chapter 8 and ensure to leave the setup name empty (only confirm with ENTER) to save the settings as the default.



plot line	etype
pixel	
line	_~~~_
smooth	
norre 🗌	

Choose between different data sets

The plot linetype will choose the type of data points:

- select "pixel" or "line" to export measured data points
- select "smooth" to export smoothed data points (with a frequency resolution defined in the SIM setup)
- select "pixel" AND "smooth" to export measured data points followed by a smoothed data table



Similarly for CV and IE, an ASCII export can be made using the code below.

#### For CV:

```
CLRSIM 'initialize SIM
ANA_OPEN_CV(65,"c:\thales\script\myscript","CV1") 'open saved CV1 file
ANA_PLOT_CV(1) 'plot CV graph
ANA_XASCII(65,"c:\thales\script\myscript","CV1") 'save CV ASCII with name CV1
```

An ASCII export is not possible with "POL measurement".

#### For IE:

```
CLRSIM 'initialize SIM
ANA_OPEN_IE(65,"c:\thales\script\myscript","IE1") 'open saved IE1 file
ANA_PLOT_IE(1) 'plot IE graph
ANA_XASCII(65,"c:\thales\script\myscript","IE1") 'save IE ASCII with name IE1
```

**ANA\_PLOT\_XX**(1) is required for the ASCII export of the CV and IE measurements.

For an ASCII export, first saving the file (MEAS\_SAVE\_XXX) is required. A direct ASCII export after measurement is not possible.





# **5** Sample scripts

In this part of the manual, different sample scripts are provided. These scripts deal with the standard tests and can be used as provided or modified to the user's desires. These scripts should provide a starting point for the users to start using the script software. The sample scripts provided below in the rest of this manual are also provided with required rule files and logo files in the folder **c:\thales\scripts\myscripts**.

# 5.1 Loop function

When a script is required to run multiple measurements until a condition is met then loop commands for-to step, next, and repeat - until come handy. The script provided below shows a script code with for-to step, next. In the script provided below

- 1. the potentiostat is turned on and a potential of -0.5 V is applied
- 2. Potential and current is measured and printed
- 3. In the loop, the potential is changed from -0.5 V to 0.5 V with a 0.1 V step
- 4. Potential and current is measured in each cycle

SCRIPT1	
GETPARAM	'get current configuration of potentiostat
Gal=0	
GAL=0	'turn potentiostat on
Pset=-0.5	'set potential to $-0.5$ V
Pot=-1	'turn potentiostat ON
SETUPECW	'apply setting provided above
POTENTIAL	'measure potential
CURRENT	'measure current
<pre>lprint("POT"), Pact</pre>	'print potential (in Z trace USB window)
<pre>lprint("CUR"),Cact</pre>	'print current (in Z trace USB window)
for Psetpoint= -0.5	to 0.5 step 0.1 'run loop for set potential from -0.5 to 0.5 V
Pset=Psetpoint	'link potentiostat potential to Psetpoint
SETUPECW	'apply setting provided above
POTENTIAL	'measure potential
CURRENT	'measure current
<pre>lprint("POT"),Pact,(</pre>	"CUR"),Cact 'print potential and current
get KEY\$	'read keyboard
if KEY\$="q" goto LOO	PEND: 'press q key to end the loop prematurely
next	'start the loop again
LOOPEND::	'loop end command
Pot=0	'turn potentiostat OFF
SETUPECW	'apply setting provided above
gotoMENU	'go to the main menu of the Script software
SCRIPT END	



#### **5.2 Series measurements**

In the folder c:\thales\scripts\myscripts\EIS-CV-POL-measurements, a script is provided with the rule files. This script deals with the different measurement methods looped in a cycle and the whole cycle is repeated 3 times producing a total of 9 files in the "measured-spectra" folder.

Initially, 3 rule files are produced for POL, CV, and EIS which contain the desired parameters for the intended measurements. The parameters for each measurement are listed below

- **POL:** Potential: 10mV, time: 60 seconds, sampling interval: 5 seconds
- **CV:** Potential range: 0 to 0.5 V, Scan rate: 100 mV/s, Samples: 1000 samples/cycle, Measure 10 cycles
- **EIS:** Potentiostatic mode, DC bias: @ OCP, Frequency range: 10 Hz to 10 kHz, Amplitude: 5mV

```
SCRIPT_PATH$="path" 'path to script
SCRIPT1
     GETPARAM ' get current configuration of potentiostat
     Gal=0 ' potentiostatic mode
     GAL=0 ' potentiostatic mode
     Pot=-1 'switch potentiostat i.e. cell state = on
     SETUPECW ' apply the settings above
     forNumber=1 to 3 'Run 3 loops
     MEAS OPEN POL(65, "path rule file", "pol") 'open pol rule file
     MEAS POL
                    'measure polarization curve
      pack pol_NAME$, using"pol-data@@",Number 'name code, for giving different name
      to the files which will be created due to loop
     MEAS SAVE POL(65, "@path save folder", pol NAME$) 'save polarization curve
      MEAS_OPEN_CV(65, " path_rule_file ", "cv") 'open CV rule file
     MEAS CV
                          'measure CV
     pack cv NAME$, using"cv-data@@", Number 'name code, for giving different name
                                                                                     to
the files which will be created due to loop
     MEAS SAVE CV(65, "@path save folder", cv NAME$)
                                                          'save CV
      MEAS_OPEN_EIS(65, "path_rule_file", "eis") 'open EIS rule file
     MEAS EIS
                                          ' measure EIS
     pack eis NAME$, using"eis-data@@", Number 'name code, for giving different name to
the files which will be created due to loop
     MEAS SAVE EIS(65, "@path save folder", eis NAME$) 'save EIS
              'turn potentiostat off
     Pot=0
     SETUPECW 'apply settings provided above
               'start next loop
     next
     gotoMENU 'go to script menu
SCRIPT END
```

In a loop script, multiple files are produced. Hence it must be made sure that all the files have different names. If the name of the files will be the same then with every loop, the

previously saved files will be overwritten by the newly saved file. For this a string (i.e., pol NAME) is used in the command given below

pack pol NAME\$, using"pol-data@@",Number

Here, the **pack** command will assign the Number value of the loop to the **pol-data@@**. This will result in the file numbers as given below

For loop 01: Number =01, measured file name is pol-data01

For loop 02: Number =02, measured file name is pol-data02

For loop 03: Number =03, measured file name is pol-data03

Besides the rule file, some additional files are also needed for the logo and the buttons in the script program. These files must always be copied in every new folder for a new script to properly run the script program. These files are named as *scr\_logo.icd*, *scr\_b1.icd*, *scr\_b2.icd* and *scr\_b3.icd* and so on. *b1*, *b2*, and *b3...* files will produce buttons for the script 1, script 2 and script 3... respectively.

# 5.3 ASCII export

In the folder c:\thales\scripts\myscripts\ASCII-export, a script is provided with the rule. The script not only carryout EIS measurement and save data but also save data in ASCII format. For ASCII export, the saved spectrum (EIS) is loaded into the SIM software and then is saved as an ASCII export. An ASCII export without initializing SIM is not possible with the script program.

```
SCRIPT PATH$="c:\thales\script\myscript\ASCII-export"
SCRIPT1
GETPARAM ' get current configuration of potentiostat
Gal=0 ' potentiostatic mode
GAL=0 ' potentiostatic mode
Pot=-1 'switch potentiostat i.e. cell state = on
SETUPECW ' apply the settings above
forNumber=1 to 3 step 1
MEAS OPEN EIS(65, "c:\thales\script\Myscript\ASCII-export", "eis") 'open EIS rule file
MEAS EIS 'measure EIS
pack eis NAME$, using"eis-data@@", Number 'Name files with different number during loop
MEAS SAVE EIS(65, "@c:\thales\script\myscript\ASCII-export", eis NAME$) 'Save
                                                                              EIS
                                                                                    file
(File 1)
CLRSIM 'Clear SIM, whatever is in SIM, clean it (initializing SIM)
ANA_OPEN_EIS(65,"c:\thales\script\Myscript\ASCII-export",eis_NAME$) 'open measure EIS
file (File 1-measured recently)
ANA XASCII(65,"@c:\thales\script\myscript\ASCII-export", eis NAME$) 'export as txt file
Pot=0
          'turn potentiostat off
SETUPECW 'apply the setting provided above
          'next loop
next
gotoMENU 'go to menu
SCRIPT END
```



## 5.4 EIS after current stabilization

In many applications, the user has to wait before the system stabilizes and then carry out the EIS measurement. With the script program, the changing variable can be used as a trigger and when the changing variable meets the user-defined limit (i.e. current or voltage stabilization) then the script program carries out the measurement. A sample script for such a process is provided in the folder C:\THALES\script\myscript\EISafter-current-stabilization. In the script below, current is measured every 500 ms and then the current stabilization is defined as the change in current between two consecutive current values is less than 100 pA. As this condition is met, the script software starts measuring an EIS.



```
SCRIPT_PATH$="c:\thales\script\myscript\EIS-after-current-stabilization"
SCRIPT1
                     'get current configuration of potentiostat
     GETPARAM
     Gal=0
     GAL=0
                     'potentiostatic mode
     Pot=-1
                     'switch potentiostat i.e. cell state = on
                     'apply the settings above
     SETUPECW
     CURRENT
                     'measure current
     lprint("current0"),Cact 'print current
     current0=Cact
                               'assign measured current name of "current0"
     pause 500
                               'wait for 500ms
     repeat
                                'start loop with repeat command
     CURRENT
                               'measure current
     lprint("current"),Cact
                               'print new current value (step A)
     trigger=abs (Cact-current0) 'get an absolute difference between both current value,
     lprint("trigger"), trigger 'print current difference, named as "trigger"
     current0=Cact 'name current measured in step A as "current0" for next loop
     pause 500 'wait 500 ms
     get KEY$ 'access keyboard
     until KEY$="q" or trigger<1e-10 'keep looping until the current difference is
          less than 100pA or key "q" is pressed
     MEAS OPEN EIS(65,"c:\path","eis") 'open EIS rule file
               'measure EIS
     MEAS EIS
     MEAS SAVE EIS(65,"@c:\path","eis data") 'save EIS
          Pot=0 'turn potentiostat off
          SETUPECW 'apply the settings above
     gotoMENU 'go to script menu
SCRIPT END
```

# 5.5 EIS at different bias potential

One pre-requisite of EIS is linearity. In EIS, a very small potential amplitude is used to ensure that only the linear response of the SUI is investigated. Due to this, multiple EIS measurements at different bias potentials are sometimes a necessity to understand the



behavior of the SUI. The sample script in this part measures EIS spectra at different bias potentials (from -0.5 V to 0.5 V – with a step of 0.1 V).

Here, only one rule file is required, which is measured at the parameters given below

Potential amplitude: 10 mV

Frequency range: 100 mHz to 100 kHz, starting frequency 1 kHz

Bias potential: -0.5 V

The rule file is opened before the first loop. In the first loop, the program has the parameters from the rule file and an EIS is measured. Afterward in the first loop, the bias potential is modified for the next loop whereas other EIS parameters stay the same as in the rule file. Then the next loop is measured and so on.

```
SCRIPT PATH$="c:\thales\script\myscript\EIS-vs-Bias-potential"
SCRIPT1
GETPARAM ' get current configuration of potentiostat
Gal=0 ' potentiostatic mode
GAL=0 ' potentiostatic mode
Pset=-0.5 'set potential of -0.5 V
Pot=-1 'switch potentiostat i.e. cell state = on
SETUPECW ' apply the settings above
MEAS OPEN_EIS(65,"c:\thales\script\myscript\EIS-vs-Bias-potential","eis-rule")
                                                                                'rule
file (out of loop)
POTENTIAL 'measure potential
lprint("Bias potential"), Pact 'print potential
             'Number defined for the loop
Number=-0.6
pause 500 'wait 500 ms
         'start loop
repeat
Number=Number+0.1
POTENTIAL 'measure potential
lprint("New Bias potential"), Pact 'print potential with name, new bias potential
MEAS EIS 'measure EIS
pack eis NAME$, using"eis data+@@@@mv",Number*1000 'file name
MEAS SAVE EIS(65, "@c: \thales \script \myscript \EIS-vs-Bias-potential \measured-
spectra", eis NAME$) 'save EIS
Biaspotential=Pact 'give applied potential the name of "Bias potential"
GETPARAM
Pset=Biaspotential+0.1 'Increase the bias potential by 0.1 V
SETUPECW 'apply the settings above
pause 500 'wait 500 ms
get KEY$ 'access keyboard
until KEY$="q" or Number>=0.5 'keep looping until key "q" is pressed or the number>=0.5
Pot=0 'turn off potentiostat
SETUPECW 'apply the settings above
gotoMENU 'go to menu
SCRIPT END
```

In the folder C:\THALES\script\myscript\EIS-vs-Bias-potential, two scripts are provided which include a "return-until" loop and "for-to (step), next" loop. Here, In

**repeat** - **until** loop, an additional **or** function is introduced. So that loop can be stopped with one of two provided conditions.

For file names, a template of <u>eis\_data+@@@@mv</u> is used. This allows the +/- sign in the name, with file numbers. The saved EIS files will have the name as

eis\_data-0500mv

eis\_data-0400mv

eis\_data+0400mv

eis\_data+0500mv

# 5.6 Potential vs time

The script shown on the next page illustrates the decay of potential with time. Here following steps are carried out

- 1. Select potentiostatic mode
- 2. Apply 1 V potential
- 3. Turn on potentiostat
- 4. Measure potential and current (and print in Z trace USB window)
- 5. Wait 1 second
- 6. Turn off potentiostat
- 7. Measure potential and current (and print in Z trace USB window)
- 8. Wait for 1 second
- 9. Start loop, measuring potential and current decay every second until the loop is interrupted with the "q" key
- 10. Save data in a text file

Measured potential is saved in a "text file" in a tabular format. For the table, a header is defined. Outmask defines the pattern in which the data will appear. Before the starting of a loop, a text file, named as test.txt is written and opened via the code

open1,65,2,"@c:\thales\script\myscript\potential-vs-time\test.txt,w"

Here, 65: PC Filesystem, 2: internal Zennium Hard disc

In folder **c:\thales\script\myscript\potential-vs-time**, two scripts file are present which contains multiple (slightly) different script codes. This is to illustrate that there are many ways to write a script for the same experiment.



```
SCRIPT1
HEADER$ ="TIME/sec
                      POTENTIAL/V" 'header for output text file
                      -#.@@@@@^^^^"'code for the number format of the data file
OUTMASK$="#######.#
CRLF$=hex$("0d0a") 'code for -> go to next line
     GETPARAM 'get active configuration of potentiostat
     Gal=0
     GAL=0 'go to the potentiostatic mode
     Pset=1 'set potential to +1 V
     Pot=-1 'turn Potentiostat on
     SETUPECW 'apply the settings above
     POTENTIAL 'measure potential
     lprint"Pot-ON=", Pact 'print potential
     pause 1000 'wait for 1 seconds
           Pot=0 ' turn potentiostat off
           SETUPECW 'apply the setting above
     POTENTIAL 'measure potential
     lprint"Pot-OFF=", Pact 'print potential and current
     pause 1000 ' wait for 1 second
      open1,65,2,"@c:\thales\script\potential-vs-time\test.txt,w"
       'create text file for writing data, "w" is used for write able file
     print#1,tcode$ (1, HEADER$)+CRLF$
'print header, tcode$ manages font of the header, CRLF$ is used to go to next line
           for t%=0 to 1000
                               'loop starting (1000 cycles)
           POTENTIAL 'mesure potential
           lprint"POT=", Pact 'print POT
           pause 1000 ' wait for 1 second
           \texttt{TIME=t\$} 'assign the <code>TIME</code> variable the same values at <code>t</code>%
           POT=Pact 'assign POT variable the value of measured potential
           packASCII$, usingOUTMASK$, TIME, POT
             'assign TIME, POT values the format defined in OUTMASK$
           print#1,ASCII$+CRLF$; 'print TIME and POT value in the table
     get KEY$ 'access keyboard
           if KEY$="q" goto LOOPEND: 'press key "q" to end loop prematurely
           next 'go to next loop
                'loop end command
LOOPEND::
close1 'close the file test.txt
gotoMENU 'go to the main menu of the script software
```

SCRIPT END