



## FlowTEK™ ver 1.5 Training Guide

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## 1. Introduction

### 1.1. *What does FlowTEK™ comprise?*

#### 1.1.1. System overview

FlowTEK™ is comprised of a combination of hardware and software components. When these are combined with the skill of the user, a powerful experimental platform and analytical system results. The hardware consists of a multi-function interface card which is installed in the computer and a proprietary distribution board which is used to connect the various manifold devices and detectors. FlowTEK™ has been applied on Desk top PCs and embedded processors such as the PC-104 and Std-32 platform. Support for Laptop computers is also available with some limitations.

#### 1.1.2. Hardware overview

The interface card allows both digital and analog input and output. FlowTEK™ makes particular use of the analog input and digital output capabilities of the interface card. Support for the digital input and analog output functionality of these interface cards is also included, though not often used. The distribution board provides a convenient means of connecting the manifold devices to the data acquisition and device control system. It also provides simple signal conditioning circuitry for the analog input and digital output.

#### 1.1.3. Software overview

FlowTEK™ allows FIA and SIA practitioners to control manifold devices using simple or complex control procedures to perform the actions required to manipulate a sample and present it to a flow-through detector. During sample manipulation in the flow-injection manifold, FlowTEK™ also provides a means of acquiring

response data and then manipulating these data to yield analytical information.

## 1.2. *Where to start*

### 1.2.1. Procedures, Methods, and Directives

The basic building blocks used in FlowTEK™ are Procedures, Methods, and Directives. These can be combined to form the simplest of single experiments or complex automated process analysis protocols.

*A Method is defined as the sequence of events necessary to obtain a single analytical result. A Method would typically consist of pump and valve actions to inject a sample and monitor its progress through the flow-through detector.*

A *Procedure* is a combination of Methods grouped together to achieve a variety of analyzer actions. Procedures allow for the automation of the entire analytical sequence required to obtain a result. It is possible to nest Procedures to obtain even more complex and powerful options. Procedures provide a means of reusing recurring Procedures in different applications with a minimum of redefining new Procedures.

A *Directive* is an instruction to the instrument, or software to perform an action. In many cases, the action achieved by a Directive can be selected by going through one or other menu option. Directives provide a means of scheduling the selection of these menu options for some time during a Procedure when you may not be present, e.g. in an automated run. Directives can be included both in Methods and Procedures.

### 1.2.2. Creating and editing a Method

Methods are created and edited on the Method Menu page. The menu options on this page are as follows:

- Configure a device - allows a user to define and add additional digitally controlled devices
- Experiment time - specifies how long the experiment is and when to start acquiring data
- Type of Devices - specifies the devices that will be controlled by FlowTEK™
- Insert an event - inserts an event for one of the devices
- Delete an event - deletes an event for one of the devices
- Startup settings for digital ports - sets the values of the digital ports on start up
- File - save, retrieve, or erase a file
- Insert Time - inserts time between events
- Delete Time - deletes time between events

### 1.2.3. Creating and editing a Procedure

Procedures are created on the Repeated Menu page.

- Build a Procedure - allows you to enter the Procedures, Methods, and Directives that will go to make up a Directive
- Display a Procedure - lists Procedures that have been built already
- Main Procedure - specifies which Procedure will begin when Go! is selected
- Go! - executes the Main Procedure
- File - specifies where the data will be stored
- Setup - defines certain parameters that are used by some of the directives.

### 1.2.4. Adding Directives to Methods and Procedures

A Directive is added to a Procedure by typing the directive number with a .DIR extension. This format is used to simplify

interpretation of the Procedure entries and does not represent a file with that name. Directive instructions are hard coded into the software. The parameter is an integer used by the Directive to signify a particular user selection.

A Directive is added to a method by specifying a Directive device. This provides a time line along which directives may be inserted. Parameters are entered after the directive has been positioned on the time line and are defined in the specific Directive description.

### 1.2.5. You try!

Create a Method with two devices, a Valco valve and Alitea pump. The experiment should be 90 seconds long with the pump being switched on at time 0 and off at time 90. The valve should be switched from the load to the inject position at time 10.

Create a Procedure which executes this method 3 times with a 1 minute pause before the three measurement.

## 1.3. *Carrying out an experiment*

### 1.3.1. Just once

After you have created a method, you can execute it and see how the various devices respond to the method. To execute a Method once, select **Once** from the Main menu. Watch the time line and compare what is happening with what you intended. While a Method is running, data are acquired from the detector. The box in the bottom right hand corner shows the time elapsed from the start of the experiment and the response. You can watch the FIA profile emerge. To overlay peaks press **Alt-O**. The frame around the profile box will change to green to indicate that Overlay is active. To de-activate it, simply press **Alt-O** again.

At the end of the experiment, FlowTEK™ will calculate the various peak parameters and display these in the Peak Parameter box.

These data will be saved in a Reduced data file. The actual detector profile will be saved in a Profile file together with the method used to obtain the profile. If you select that the Abridged Profile file should be saved, then a file will be created with just the profile data and all the other data used to specify the instrumental conditions for that specific experiment will be omitted. This file is useful when you want to import the profile into a third party package.

### 1.3.2. Repeatedly

You can Repeat a Method by building a Procedure. A simple Procedure may contain one line that instructs FlowTEK™ to repeat the Method 10 times. The Repeated Menu page allows the creation of Procedures. The Display menu option displays any previously define Procedure. You Build a Procedure by giving it a name and then entering the Methods, Procedures, and Directives that you want to include in the Procedure. You can nest up to 10 levels of Procedures. Each Procedure can have as many as 20 instructions. To display a list of defined Procedures and Methods press F10. You must tell FlowTEK™ what the Main Procedure is. This is the Procedure that will be executed when you press Go! When the Main Procedure is completed the computer will Beep and wait for the next user input. The File menu option allows you to specify the file names of the Reduced data and Profile files.

You can abort a Method or Procedure at any time by pressing Alt-Q. Pressing Esc will abort at the end of the Method or skip to the next step in a Procedure if a Wait is in progress.

### 1.3.3. You try!

Execute the Method once. Then switch to the Repeated menu page. Specify the Procedure which you defined in the last exercise as the Main Procedure. Save the Reduced data and Profiles data in appropriate files. Execute the Procedure and follow as the Procedure is executed.

## 2. Basic principles of operation

### 2.1. Examining your data

#### 2.1.1. Profiles

The FIA / SIA response profiles provide important information about the experiment being carried out. With experience, the FIA worker will learn to interpret the shape of the profile. Also by comparing profiles of successive experiments, you can go a long way towards judging whether an experiment has been successful or not.

One way of comparing profiles is to overlay them. This is achieved by pressing Alt-O.

#### 2.1.2. History

The History menu page provides a trend of the results obtained in up to 100 experiments. On this page, it is possible to display Height, Area, Peak time, Peak Width at a particular Height, and Concentration. These data can either be displayed as dots (selected with a .) or bars (selected with a / or \). You can also examine the profiles of any selected experiment by selecting it and choosing the Profile menu option. When you select a particular experiment, all the peak parameters will be displayed in the Peak parameter box.

You can swap to this page during a Procedure by pressing Alt-T.

#### 2.1.3. The Note Pad

The Notepad provides a summary of all the User-selectable menu options. This is most useful during trouble shooting to identify whether the parameters are as you wanted them to be. You can also use menu options on this page to print out Methods,

Procedures, or a hard copy of the experimental settings used in a particular experiment.

#### **2.1.4. Using third party packages**

All data files used in FlowTEK™ are saved in ASCII format and therefore lend themselves to being imported into third party statistical, graphing, or data analysis packages.

#### **2.1.5. You try!**

Open a window to view the Profile of your second experiment. View your data on the History page and trying loading a Profile. Try importing the reduced data file into the DOS Editor.

## **2.2. Calibration**

### **2.2.1. The Calibration Response Table**

Data used to calculate calibration constants are stored in a Calibration Response table. This table has 9 rows and 3 columns. The response (Height, Area, Time, or Width) for a particular concentration are stored in the Rows of the table. Replicated values are placed in each column. FlowTEK™ keeps a track of the number of replicates. When you measure more than three replicates, the oldest datum is replaced by the newest value. The regression is carried out on a simple arithmetic mean of the data for a particular concentration.

Before a Calibration calculation can be completed, you must specify the first and last standards in the Calibration Response Table. This means that it is possible to store the data for more than one calibration graph in the Calibration Response Table. Consider the following example Calibration Response Table.

Conc	1 <sup>st</sup>	2 <sup>nd</sup>	3 <sup>rd</sup>	Avg
2.0	2.13	2.02	2.09	2.08
4.0	4.25			4.25
6.0	5.98	6.25		6.12
20.0	5.82			5.82
40.0	9.82			9.82
60.0	15.75			15.75

The data in the first three rows could be for one manifold, and the data in rows 5 to 7 could be for another analyte or a manifold which gives less sensitive readings. From FlowTEK™ point of view, it is perfectly acceptable to have a different number of replicates for one calibration set. In each case, the calibration algorithm works with the mean. To calculate the regression constants for the first data set, specify the first standard as 1, the last as 3, and then select a calibration model. To calculate the regression constants for the second data set, specify the first standard as 4 and the last as 6. Of course you can have any number of standards (up to 9) for a particular calibration set.

### 2.2.2. Entering data

There are two ways of entering data into the Calibration Response Table. The one is simple manual entry using the Edit, Insert, and Delete menu options. Use the Insert menu option to create a new standard. You can only Edit existing data. Use the Delete menu option to delete a standard. The second option is to use Directives. This option will be discussed in more detail later.

### 2.2.3. Calibration models

You can select one of six calibration models to apply to the calibration data. They are linear ( $y = a_1x + a_0$ ), quadratic ( $y = a_2x^2 + a_1x + a_0$ ), trinomial ( $y = a_3x^3 + a_2x^2 + a_1x + a_0$ ), exponential

( $y = ae^{bx}$ ), and rectangular hyperbola ( $y = a_0/(a_1 + x)$ ). The latter two are calculated by performing a translation on the data which converts the functions into linear functions. The sixth option applies a cubic spline function. The seventh option allows you to perform the first five regression calculations and select the one which provides the best correlation coefficient ( $r^2$ ), i.e. closest to 1.0.

#### 2.2.4. You try!

Enter the data for the first three standards given in the table above. Set up the first and last standard numbers and select the linear memory model and take note of the way that the spread of data for the first and third standard is represented. Take note of the correlation coefficient and see how it changes as you select other regression models.

### 3. Advanced Features

#### 3.1. *Connecting Devices and Detectors*

##### 3.1.1. Digital outputs (Switch or TTL)

Devices are controlled by either digital or serial commands. Serial devices are linked to the serial port on the computer and the serial port is activated using Directives which will be discussed later. Digital devices are connected to one of the eight digital outputs on the Distribution box. These connection can be tested by setting up one of the function keys (**F3** to **F9**) with the appropriate signal. This setup is achieved on the Setup Menu page using the Function keys menu option.

The digital outputs can be configured as Switch i.e. open circuit (floating voltage) or closed circuit (0 V) or TTL i.e. high (5 V) and low (0 V). This selection is made on the distribution board with jumpers. Refer to the instruction manuals for the specific device for the most appropriate selection.

##### 3.1.2. Analog inputs

The response from the detector is monitored using one of the four 12 bit analog input ports. The first two have amplifier circuitry on the distribution board. The second two pass the 0 to 10 V signal directly to the interface board. In addition to amplifying the signal, it is possible to remove and offset of  $\pm 12$  V and also apply one of there levels of electronic filtering. The manual describes how these facilities are activated.

You can monitor the input on the analog input channels by pressing F1. This will give the actual voltage seen by the A to D converter, i.e. after amplification, and the Response after applying the Response function. The response function is selected on the Setup Menu page under the Detector Menu option. The options

are log, - log (e.g. pH), first derivative, Inverse (10.0 - Response), None, and D3 (1.0-Response).

### **3.1.3. You try!**

Program two of the function keys to switch the valve to the Inject and Load position. The digital signal for one position is 01 and for the other 10. (You can enter binary numbers by prefacing the number with a B.) See whether you have programmed them correctly by calling up the Notepad page. Try the function keys out to see if they do what you expect they will.

See what voltage is being received by the A to D converters by pressing F1 on the Main Menu page.

## **3.2. User Configuration**

### **3.2.1. Setting up Detector parameters**

There are several user selectable options available for the detector(s) you have linked to FlowTEK™. These are setup on the Setup Menu page and include the input port, response function, auto zero strategy, width at which height is measured, time at which peak height is determined, time period for which the area under the profile is determined, and Time at which data collection should commence (set up on Method Menu page). The present value for each of these is displayed on the Note Pad menu page. Make sure that you understand the implications of each of these settings.

Before you can make these selections you will need to read up on the output from the detector in the detector manual. You may even have to measure the output using a multi meter.

### 3.2.2. Setting up Device parameters

If you want to add a device to the device table, you must first establish what actions you want to have FlowTEK™ perform (3 max.) and then establish what digital signals are required to achieve this. The Config Device menu option on the Method Menu page is used to add a new device. Before you add a new device, make sure that you are not over writing a device which you are still using by looking on the Notepad page to what the existing device definitions are.

The first action that you define will be reflected above the line on the time line. These second will be reflected below the line and the third will be reflected on the baseline of the time line. Each of the hot keys used to specify a device must be unique for the device. The manual provides additional information on setting up devices.

### 3.2.3. More about Directives

In the Appendix of the manual and one of the chapters, all of the directives are listed and described. Review them with your trainer and ensure that you understand all of them.

Dir	Description	Parm	Description	Def
32	Additional diagnostic data	0	No	0
		1	Yes	
33	Select printer on	0	Printer Off	0
		1	Printer On	
34	Select COM port and baud rate	0	Disable Serial COMS	1 & 96
		1	COM1	
		2	COM2	
		3	COM3	
		4	COM4	
		12	1200 baud	
		24	2400 baud	
		96	9600 baud	
35	Check Correlation coef	0	Accept if $r^2 > 0.0$	0
		1	Accept if $r^2 > 0.98$	
		2	Accept if $r^2 > 0.99$	
		3	Accept if $r^2 > 0.999$	
36	Select detector channel	1-4	Channel Number	1
37	Follow peak or valley	0	Valley	1
		1	Peak	
38	Concentration data format	0-4	No. of decimal places	3
39	Time to start measurement	0-999	Time in minutes	0
40	Time to start measurement	0-999	Time in seconds	0
41	Time for AutoZero	0-999	Time in seconds	0
42	Analog output based on the Set Point concentration	1-2	Analog output channel	1
43	Analog output to channel 1	0-100	Voltage output * 10	0
44	Analog output to channel 2	0-100	Voltage output * 10	0
45	Analog output based on response	1-2	Analog output channel	1
46	Compare to Setpoint - Warn			
47	Compare to Setpoint - Alarm			
48	Compare to Check std			
49	Allocate standard response	1-16	Std number	1
50	Clear calibration response table			

Dir	Description	Parm	Description	Def
51	Select First Standard	1-16	First Std number	1
52	Select Last Standard	1-16	Last Std number	3
53	Regression Model	1	Linear	1
		2	Quadratic	
		3	Trinomial	
		4	Rectangular hyperbola	
		5	Exponential	
54	Wait for x min	0-999	No of minutes	0
55	Wait for x seconds	0-999	No of seconds	0
56	Wait for digital input High	1-4	Input point	1
57	Wait for digital input Low	1-4	Input point	1
58	Wait for keypad input	0-9	Key on keyboard	0
59	Digital output to port 1	0-255	Value to output	0
60	Digital output to port 2	0-255	Value to output	0
61	Output a character to the serial port	0-255	ASCII Value to output	0
62	Select acceptable baseline noise level	0-1000	Noise (in mV) 0 disable checking	0
63	Select amount of output damping	0-10000	Maximum change in voltage Damping (mV) 0 disables damping	0
64	Calculate and print the last response			
65	Select peak parameter for calibration response table	0	Height	0
		1	Area	
		2	Width	
		3	Time	
66	Output a string to the serial port	0-255	Command number in SER.CFG	0
70	Select Instrument Diagnostics	0	Disable diagnostics	0
		1	Enable diagnostics	
72	Generate a Warning if Digital Input High	0-4	Digital Input Point	0
73	Generate a Warning if Digital Input Low	0-4	Digital Input Point	0

Dir	Description	Parm	Description	Def
74	Generate a Alarm if Digital Input High	0-4	Digital Input Point	0
75	Generate a Alarm if Digital Input Low	0-4	Digital Input Point	0
76	Generate a Warning if Peak height drops below specified limit	0-10000	Peak height in mV	0
80	Perform a Procedure or Method based on Digital Input	0-999	Procedure Number	0
81	Smooth the Analog input	0-2	0 – No smoothing 1 – Moving average 2 – Savitzky Golay	0
82	Set Analog Input range	0-1	0 – 0 to 10V 1 – -5 to 5V	0
83	Set up Digital Output mask	0-1024	Mask value	0
84	Clear Digital Output bit	1-12	Bit to clear	0
85	Set Digital Output bit	1-12	Bit to set	0
254	Reset Micro			

### 3.3. Using Directive 66

Directive 66 is used to send serial commands to the selected COM port. All possible serial strings that can be sent are stored in the SER.CFG file. This ASCII text file has the format shown in the following table. Additional serial strings can be added using any text editor such as Notepad or Edit. Command numbers must be in the range 0 to 255. The following Table lists your SER.CFG file as it stands when the system is delivered.

Cmd No	Serial String	Description
1	/YGO1	Selvalve_pos1
2	/YGO2	Selvalve_pos2
3	/YGO3	Selvalve_pos3
4	/YGO4	Selvalve_pos4
5	/YGO5	Selvalve_pos5
6	/YGO6	Selvalve_pos6
7	/YGO7	Selvalve_pos7
8	/YGO8	Selvalve_pos8
9	/YGO9	Selvalve_pos9
10	/YGO10	Selvalve_pos10
11	/1S11R	Speed52.5rpm
12	/1S12R	Speed45rpm
13	/1S13R	Speed37.5rpm
14	/1S14R	Speed30rpm
15	/1S15R	Speed22.5rpm
16	/1S16R	Speed15rpm
17	/1S17R	Speed7.5rpm
18	/1S18R	Speed7.125rpm
19	/1S19R	Speed6.75rpm
20	/1S20R	Speed6.375rpm
21	/1S21R	Speed6rpm
22	/1S22R	Speed5.625rpm
23	/1S23R	Speed5.25rpm
24	/1S24R	Speed4.875rpm
25	/1S25R	Speed4.5rpm
26	/1S26R	Speed4.125rpm
27	/1S27R	Speed3.75rpm
28	/1S28R	Speed3.375rpm
29	/1S29R	Speed3rpm
30	/1S30R	Speed2.625rpm
40	/1A0R	Pump_Forward
41	/1D0R	Pump_Reverse
42	/1TR	Pump_Stop
43	/1ZR	Pump_Reset
50	/ZGoA	Inj_Valve_Position_A

Cmd No	Serial String	Description
51	/ZGoB	Inj_Valve_Position_B

### **3.4. Command line options**

The command line is used to pass important information to the program before it starts up. There are three command line switches. The first specifies which interface card you are using (Eagle PC-30B, RTD ADA2100 series, National Instruments PCMCIA, or PC104). The second specifies the DMA channel used for analog input (1 or 3). The third specifies the procedure which will be executed on Startup if a key is not pressed while the Title Screen is visible. You can use an empty procedure. A typical command line sequence would be `flowtek /n /1 nop.pdr` and this is frequently setup in a batch file called `ft.bat`.

## 4. Notes

