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A DIGITAL "BOXCAR INTEGRATOR" FOR IMS SPECTRA

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When trying to detect or quantify a signal at or near the limit of detectability, it is invariably embeded in the noise. This statement is true for nearly all detectors of any physical phenomena and the limit of detectability, hopefully, occurs at very low signal-to-noise levels. This is particularly true of IMS (Ion Mobility Spectrometer) spectra due to the low vapor pressure of several chemical compounds of great interest and the small currents associated with the ionic detection process.

Gated Integrators and Boxcar Integrators or Averagers are designed to recover fast, repetitive analog signals. In a typical application, a time "Gate" or "Window" is generated, characterized by a set delay from a trigger or gate pulse and a certain width. A Gated Integrator amplifies and integrates the signal that is present during the time the gate is open, ignoring noise and interference that may be present at other times. Boxcar Integration refers to the practice of averaging the output of the Gated Integrator over many sweeps of the detector. Since any signal present during the gate will add linearly, while noise will add in a "random walk" fashion as the square root of the number of sweeps, averaging N sweeps will improve the "Signal-to-Noise Ratio" by a factor of the square root of N.

Many detection algorithms are in use today in various instruments. The simplest ones quantitize the signal from the IMS cell and then respond to the amplitude of a single largest data point within a fixed "window" or group of data points following each trigger pulse. Fundamentally, all detection algorithms, simple or sophisticated, are band pass filters designed to provide some attenuation to the noise frequencies involved with little attenuation at the signal frequencies involved. Improvement of the Signal-to-Noise Ratio will lower the minimum quantity or concentration of chemical vapors that can be detected. Multiple filtering occurs because there are several frequency bands involved in real world measurements.

The first filter section is inherent in the frequency response of the electrometer detector and any analog signal amplification prior to digitizing the ion spectrum. This is usually a low pass filter with a corner frequency of several kilohertz. The spectrum is then digitized. Figure #1 shows the typical single sweep background noise in the region where detected chemicals may appear. Figure #2 shows an idealized chemical signal ion peak. It would be superimposed on the noise signal. At the limit of detectability, it may be smaller in amplitude than the noise signal. Furthermore, if it is a real chemical signal, it will grow slowly for tens of sweeps, hold for a few more, and finally decay, frequently at a slower rate which yields a tail. This provides several opportunities to further filter the signal using different criteria. How wide (milliseconds or number of channels) is a typical ion peak in a spectrum? How long (seconds or number of sweeps) is the chemical present in the detector?

Our new computer program, KEY3, differs from earlier digital programs in several important respects. Indeed, it emulates the best features of the older analog Boxcar Integrator technology, in what we believe are novel ways.

If the operator preselects the chemical detection windows (up to 10) and background windows (up to 2) the program operates upon raw data from each and every sweep. This data may be stored on disk independently of the full spectrum storage. Thus the chemical detection or quantitation is separated from full spectrum averaging and storage criteria allowing independent parameter adjustments. The detection program can also be run or rerun from stored data, but for this analysis I will consider the case of real time raw data.

In Figure #3 the noise of Figure #1 and the signal of Figure #2 are added, thus showing what each sweep looks like prior to analysis. The signal window is centered over the drift time of the chosen chemical. The background windows are normally set to quiet regions of the spectrum before and after the signal window. We recommend that all window widths be set to about 110% of the IMS gate width to maximize the Signal-to-Noise Ratio of the data. The Signal Recovery Equations are shown in Figure #4. All of the data points within the windows are averaged, the two background window averages are averaged together and subtracted from the signal. This results in a single number, I_k , for each sweep, which represents the amplitude of the ion peak above background. This number is effectively the output of a band pass filter, since the background subtraction eliminates the DC response of the circuit. The upper corner frequency of the filter section is about 1 kilohertz and is tuned by the window width. The wider the window width, the lower the corner frequency of the filter. Essentially, this filter is optimized for the width of the ion signal in the IMS spectrum.

In Figure #5 we leave the drift time spectrum and consider another frequency domain, that of the chemical concentration in the IMS cell plotted against sweep number. The time axis may represent tens of seconds and hundreds of sweeps depending upon the Repetition Period of the IMS detector. The detected signal near the limit of detection is, by definition, small and hence noisy. Further smoothing is required to bring the signal out of the noise for reliable detection. Three of the smoothing functions commonly used in commercial programs are:

- Moving Average
- Weighted Moving Average
- Exponential average

In the moving average, one selects the number of data points to average and all data points have equal weight. In the weighted moving average one again selects the number of data points to average, but the most recent data point carries the most weight, since from the oldest to the newest, the weight of each point is 1, 2, 3,···, n.

Figure #6 shows the equations used for exponential averaging. Several commercial instruments use the first equation where the Time Constant is selected. Other programs use the second equation where the Damping Factor is operator selected. Both equations are equivalent where the Time Constant (T) and the Damping Factor (DF) are related as shown. We chose to implement our KEY3 program with the first equation based upon setting a time constant where $1.0 \geq T \geq 1024$. A_k is the most recent averaged output while I_k is the most recent input data point.

In Figure #7 we have shown equations for these three smoothing functions with certain parameter inputs. The number of points selected for each type of moving average and the time constant used for the exponential average were selected so that the most recent input, I_k, was 25% of the averaged output, A_k.

In Figure #8 we have evaluated these equations for certain parameter values. The weight of the seven most recent data points is given for each of the three functions. All three functions average or smooth the input data. They differ only in the relative weight that they give to the individual input data points making up the output of the circuit or function.

The response of these three functions, with the previously selected parameters, to a step input is plotted as Figure #9. It is evident that the moving average function exhibits the highest frequency response, the fastest convergence and is the poorest noise filter. The exponential average function has the poorest high frequency response, the slowest convergence and is the best noise filter of the three. Consequently, we have chosen to implement the exponential average smoothing function in our KEY3 program. The largest time constant (T) is selected that will allow nearly full response of the circuit to the chemical signal in typically 3T or 4T. The longer the signal is present, the greater the value of T that can be used.

From analog filter theory we understand that the high frequency response of the Exponential Average function rolls off at 6 db per octave above the corner frequency. We know that similar multiple filter sections roll off at 12, 18, ··· db per octave and, as shown in Figure #10 and that the effective time constant grows as the square root of the sum of the squares. Therefore four filter sections with T = 2 have a rise time similar to a single filter section with T = 4, but exhibit a sharper cutoff of 24 db/octave above the corner frequency. Hence multiple filter sections exhibit a greater reduction in high frequency noise for similar response to the signal frequency of the detected chemical as compared to single filter functions.

In Figure #11 we have plotted the exponential average response of four iterations with T = 4 and the response of one iteration with T = 8 to a step input. Note that the 10% to 90% Rise Time is essentially the same and that both converge within 2% after the same number of sweeps.

In Figure #12, using the same parameters, we plot these responses to an impulse. Note that the four iterations with T = 4 produce only half the output response of the single iteration with T = 8. The high frequencies inherent in the impulse driving function are more effectively filtered out with the multiple iterations.

In actual tests of an IMS explosive detector, we have demonstrated that a two stage analog "Boxcar" Exponential Signal Averager with background subtraction was able to reduce the Minimum Detectable Concentration of TNT to one half of the best values previously obtained. We would expect that the new digital KEY3 Data Acquisition and Reduction Program will do even better, since the number of iterations (filter sections) is so much greater, parameter settings are so much more flexible and the experiment can be rerun from disk memory to optimize the settings.

In summary, our new KEY3 Data Acquisition and Data Reduction Program allows signal averaging and storage of IMS spectra in the conventional manner. It also allows real time integration of selected drift time peaks within windows, with or without background substraction. For best quantitation or alarm results at low chemical concentrations, the window width for each chemical/background should be set to about 110% of the gate width. Thereafter, the integrated "signal" can be processed by an exponential signal averaging function having a time constant of 25 to 35% of the rise time of the detected chemical. The best reliability of quantitation or alarm will occur if multiple recursions are made using a per iteration time constant that is the desired time constant divided by the square root of the number of recursions.

The specifications of our Peak Alarm/Monitor (PAM) follow.

KEY3 PROGRAM

PEAK ALARM/MONITOR (PAM) SPECIFICATIONS

- Number of Active Windows: 0 to 12
    - 0 to 10 Signal Windows
        - All with Digital Output Alarm Lines
        - Two with 0 to 10 volt, 11 bit Analog Output Lines
    - 0 to 2 Background Windows
- Window Width (PAM width): $1 \geq W \geq 55$ Dwell Channels (odd integers only)
- Exponential Divisor (Time Constant): $1.0 \geq T \geq 1024$
- Recursion (Number of Filter Sections): $1 \geq R \geq 1024$ (integers only)

ONE SWEEP

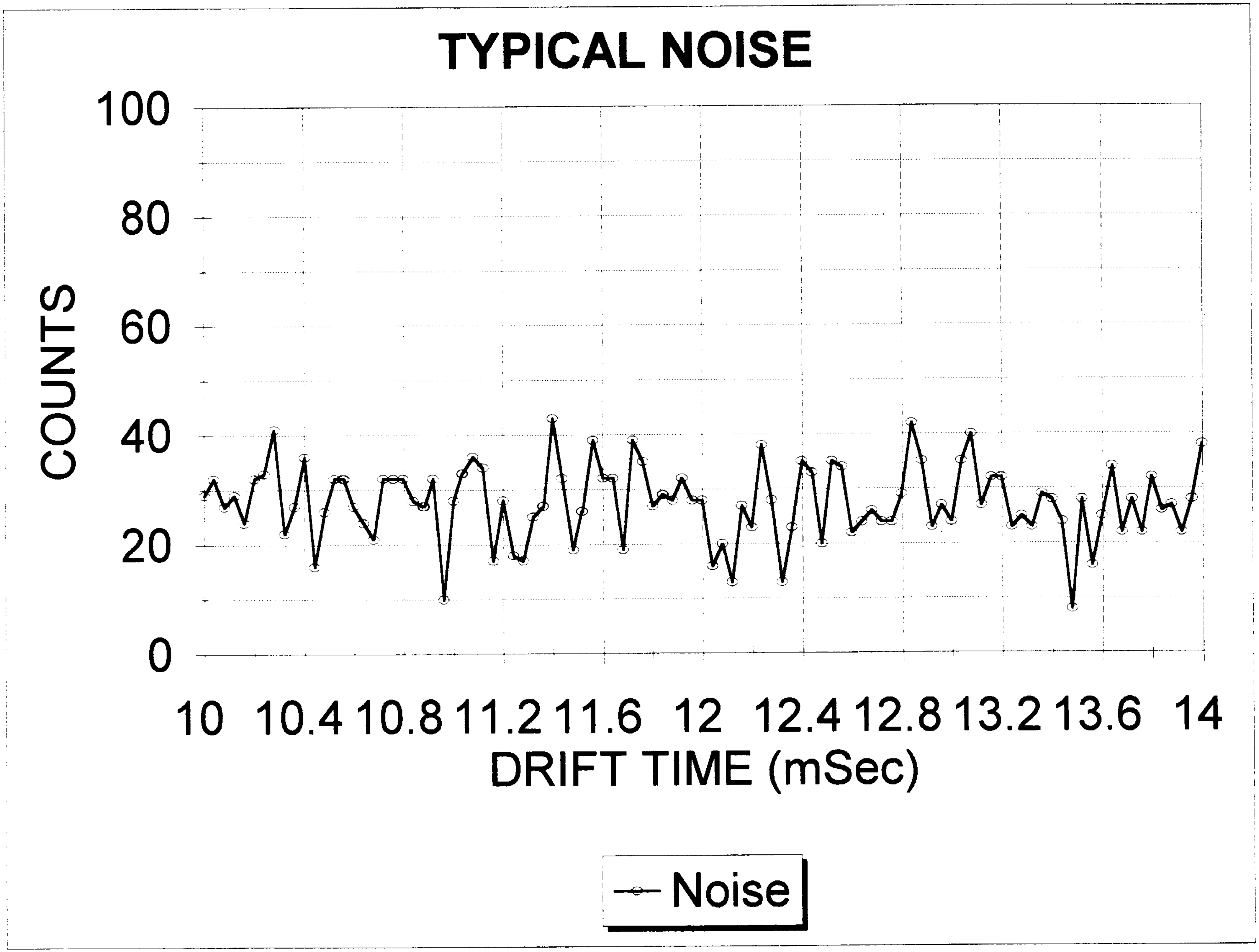


FIGURE No. 1

ONE SWEEP

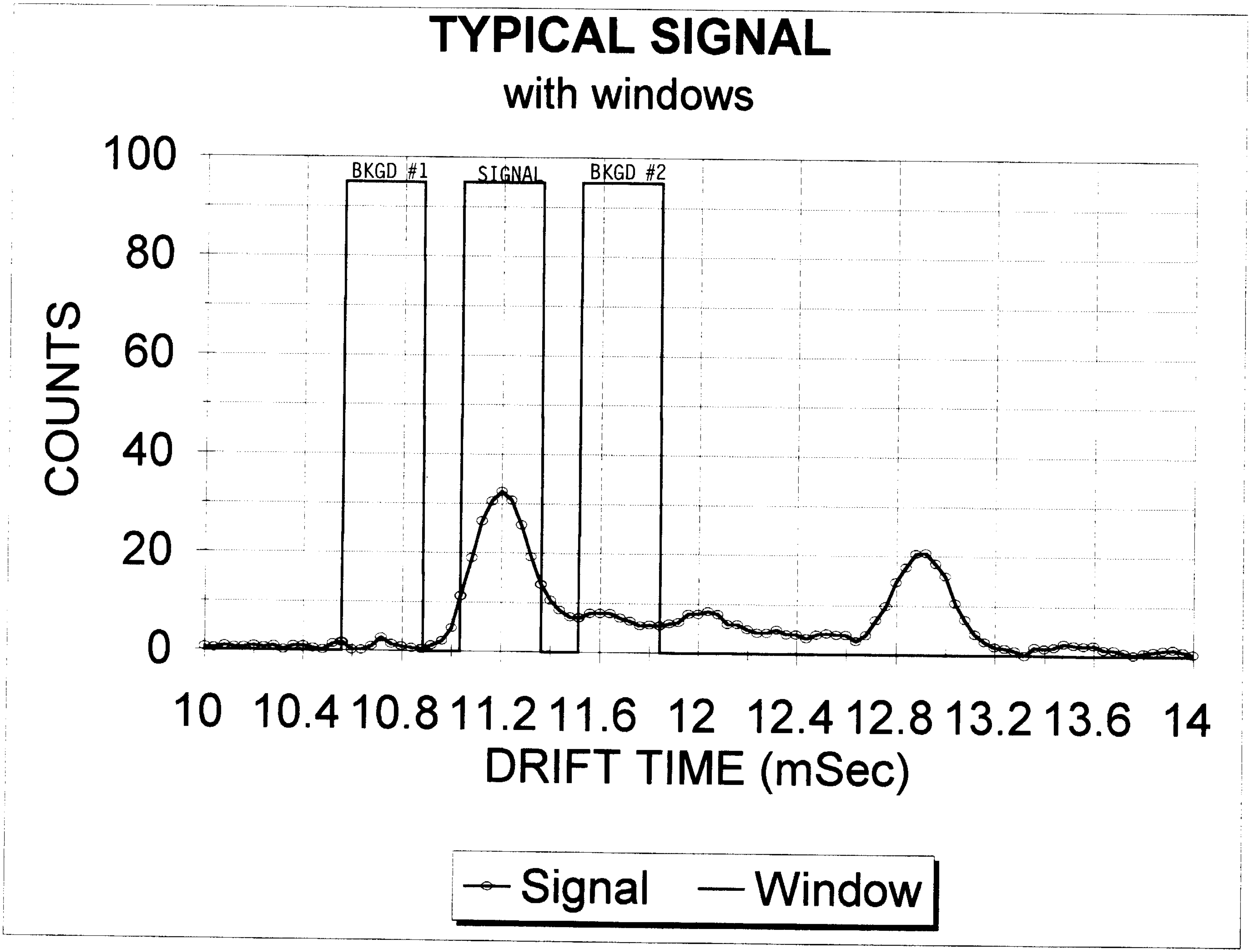


FIGURE No. 2

ONE SWEEP

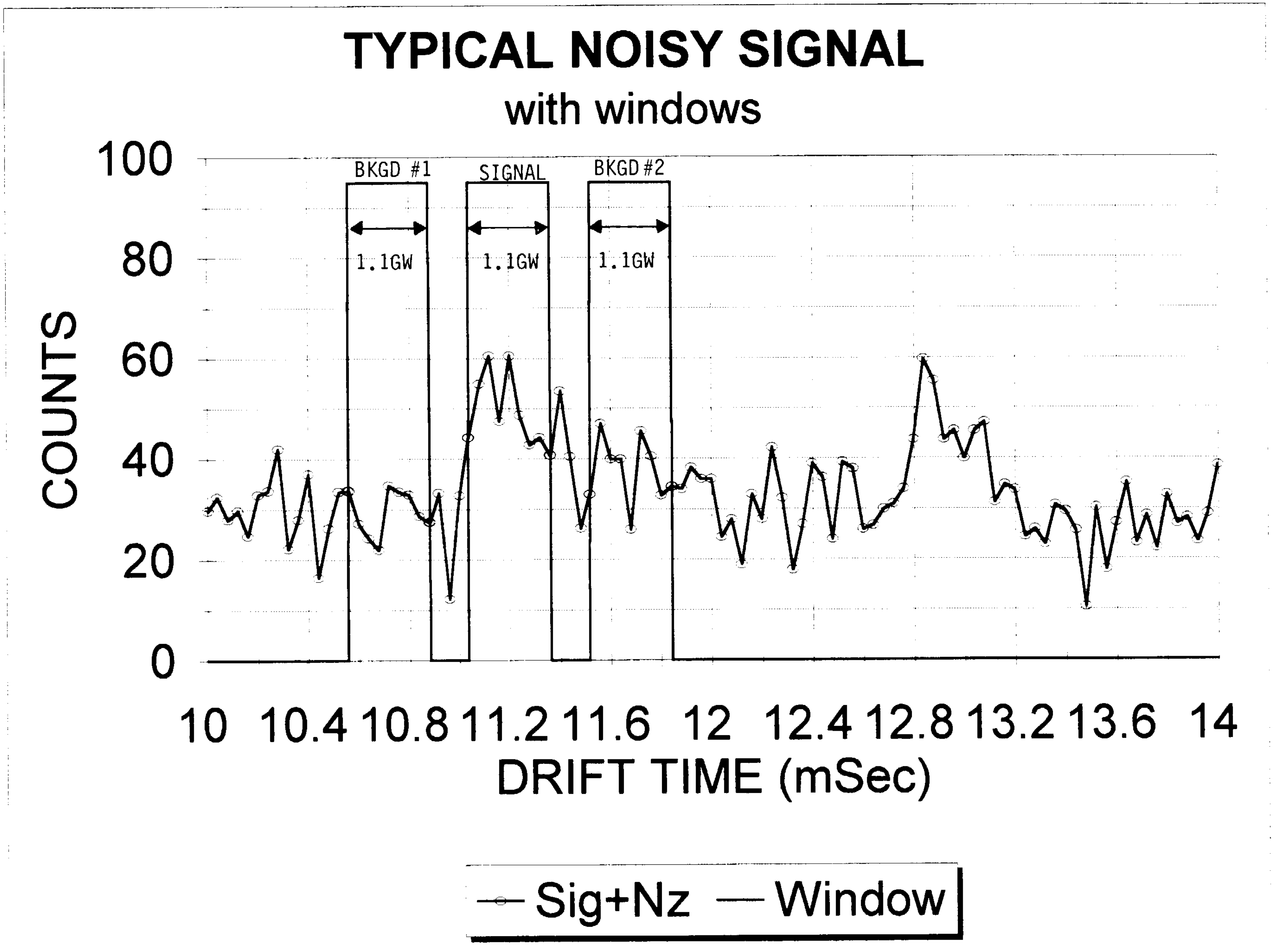


FIGURE No. 3

SIGNAL RECOVERY FROM IMS SPECTRUM

- Window Width = odd No. of channels - Centered on Ion Peak
- Best S/N: WW = 1.1 * GW
- Within Window: $Avg = [Y_1 + Y_2 + Y_3 + \cdots Y_n]/n$
- Three Averages: Signal, Background 1, Background 2
- Calculate after each Sweep:

$$I_k = \text{Signal} - [(\text{Bkgd } 1 + \text{Bkgd } 2)/2]$$

- I_k is Avg Signal above Avg Baseline, new each sweep

FIGURE No. 4

SIGNAL-BACKGROUND

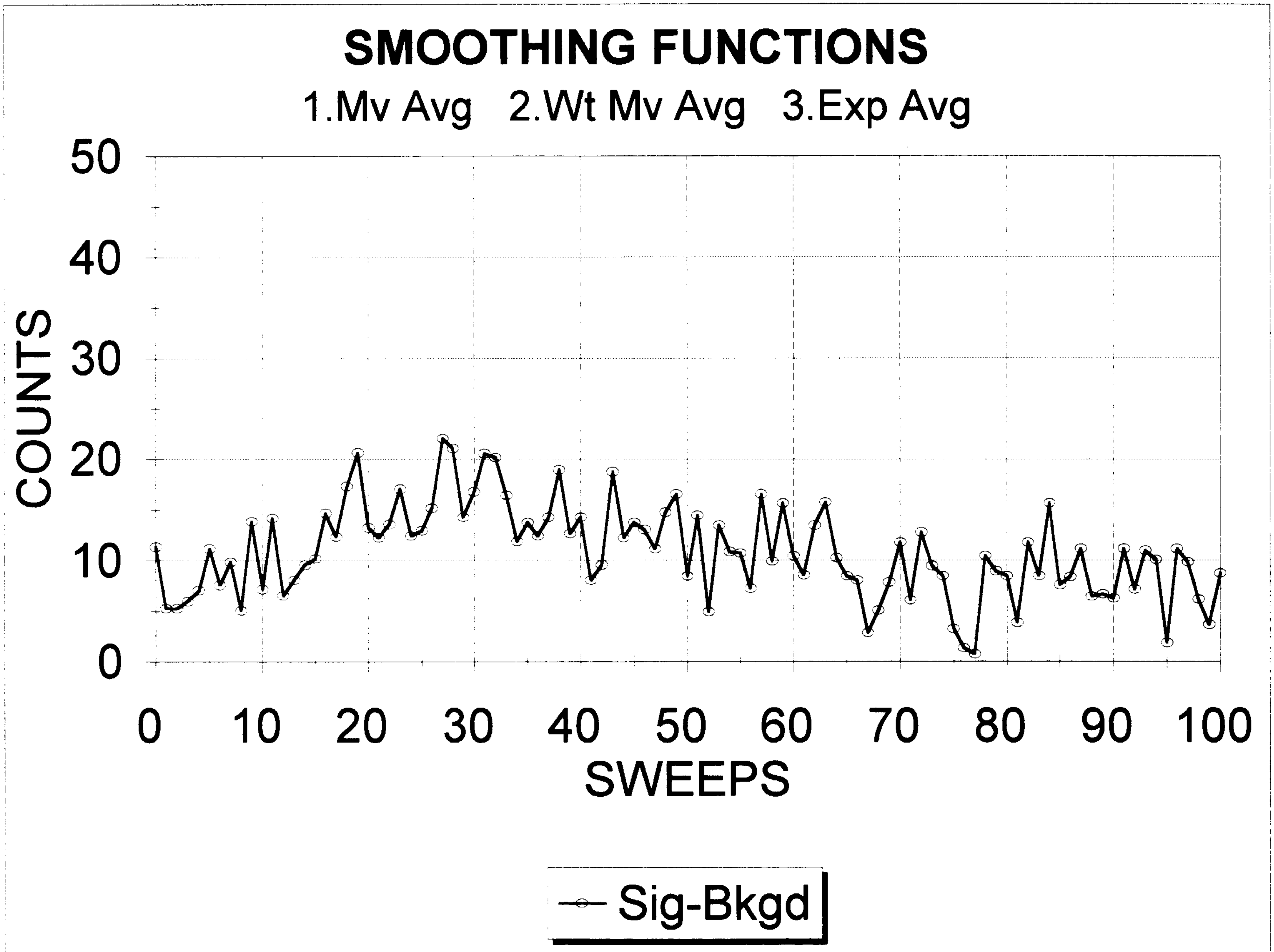


FIGURE No. 5

EXPONENTIAL AVERAGING (SMOOTHING) EQUATIONS

$A_k = A_{k-1} + [(I_k - A_{k-1})/T]$ where T = Time Constant (No. of Sweeps)

$A_k = [(DF) * A_{k-1}] + [(1-DF) * I_k]$ where DF = Damping Factor

$$DF = (T - 1)/T$$

$$T = 1/(1 - DF)$$

For KEY3 Program $1.0 \le T \le 1024$

FIGURE No. 6

GENERAL AVERAGING (SMOOTHING) EQUATIONS

1) Moving Average of 4 Points:

$$A_k = [I_k + I_{k-1} + I_{k-2} + I_{k-3}]/4$$

2) Weighted Moving Average of 7 Points:

$$A_k = [7I_k + 6I_{k-1} + 5I_{k-2} + 4I_{k-3} + 3I_{k-4} + 2I_{k-5} + I_{k-6}]/28$$

3) Exponential Averaging with T = 4, DF = 75%:

$$A_k = [I_k + (3/4)I_{k-1} + (9/16)I_{k-2} + (27/64)I_{k-3} + (81/256)I_{k-4} + (243/1024)I_{k-5} + (729/4096)I_{k-6} + \cdots]/4$$

FIGURE No. 7

GENERAL AVERAGING EQUATIONS TABLE

	I_k	I_{k-1}	I_{k-2}	I_{k-3}	I_{k-4}	I_{k-5}	I_{k-6}	Bal.	No. Sweeps to Converge
1) MOVING AVERAGE (Pt = 4)	.250	.250	.250	.250	-	-	-	.000	4
2) WEIGHTED MOVING AVERAGE (Pt = 7)	.250	.214	.179	.143	.107	.071	.036	.000	7
3) EXPONENTIAL AVERAGE (T = 4)	.250	.188	.141	.105	.079	.059	.044	.134	26
SUM 1: MOVING AVERAGE	.250	.500	.750	1.000	1.000	1.000	1.000	1.000	
SUM 2: WEIGHTED MOVING AVERAGE	.250	.464	.643	.786	.893	.964	1.000	1.000	
SUM 3: EXPONENTIAL AVERAGE	.250	.438	.579	.684	.763	.822	.866	1.000	

FIGURE No. 8

THREE AVERAGING (SMOOTHING) FUNCTIONS

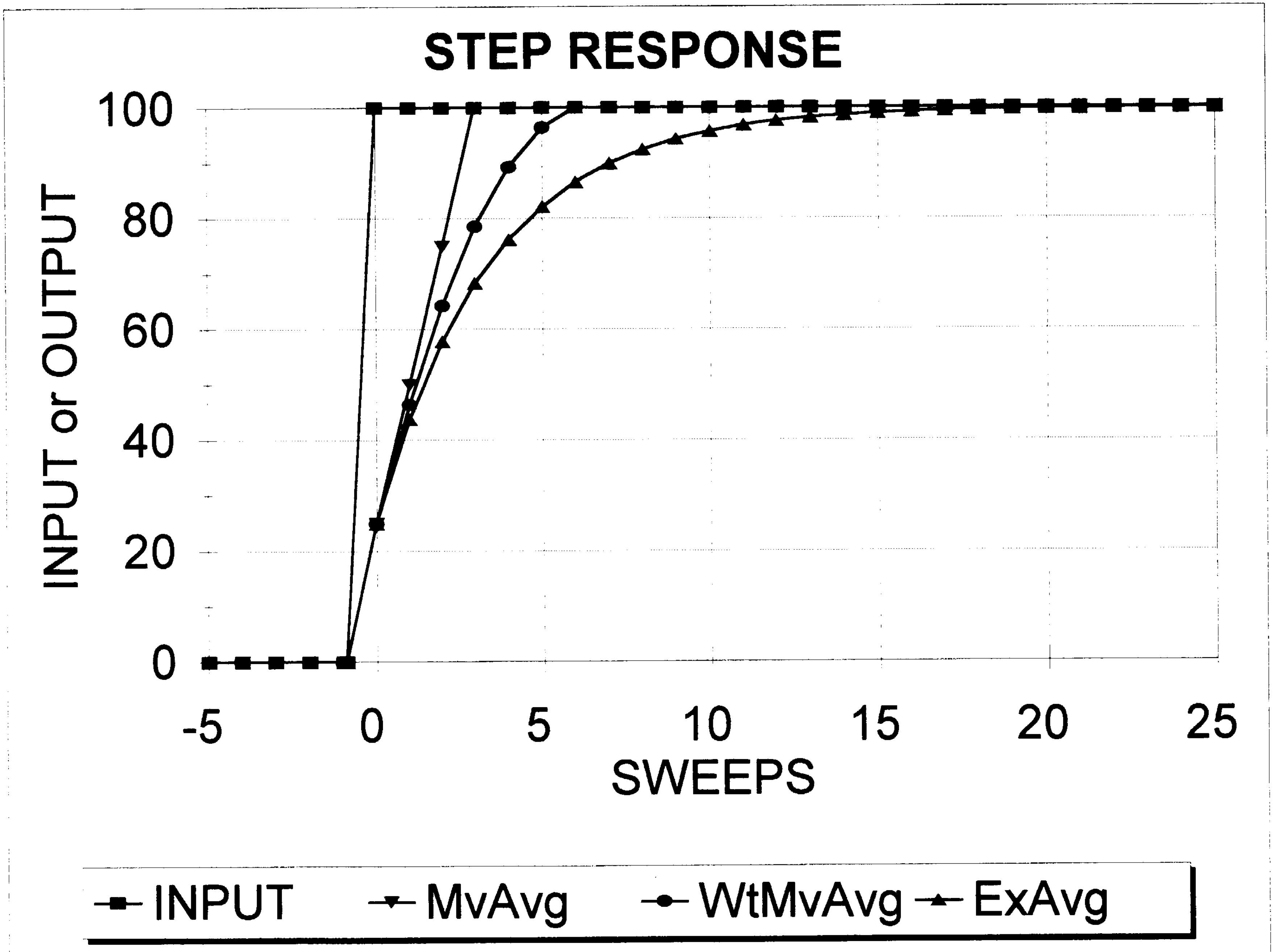
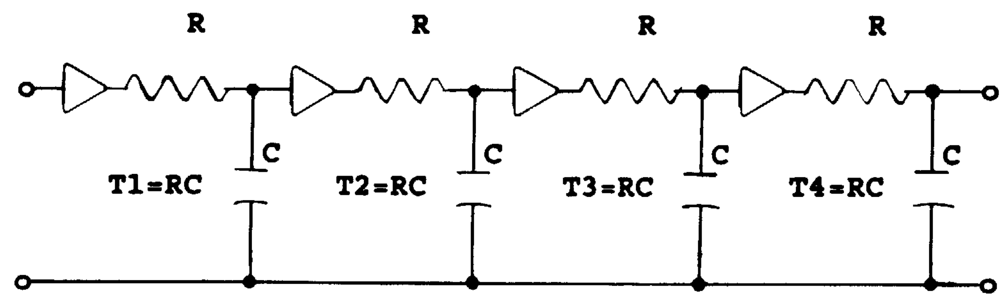


FIGURE No. 9

ANALOG RC EXPONENTIAL AVERAGING EQUATIONS WITH TABLE



$$T = \sqrt{(T1)^2 + (T2)^2 + \cdots}$$

T1	T2	T3	T4	T	DF
2	-	-	-	2	50%
2	2	-	-	2.83	64.6%
2	2	2	-	3.46	71.1%
2	2	2	2	4	75%

FIGURE No. 10

SINGLE SECTION vs EQUIVALENT 4 SECTION FILTER

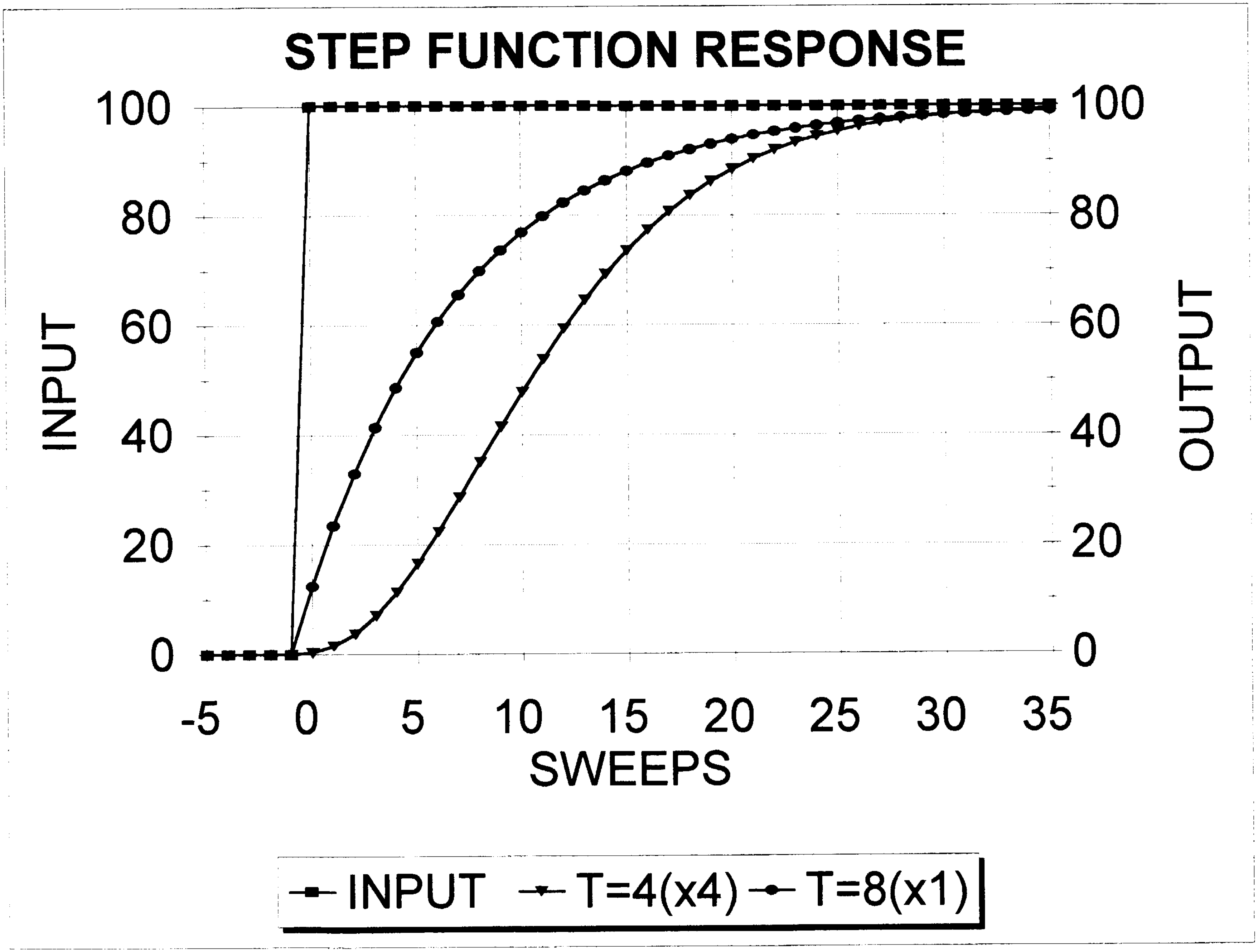


FIGURE No. 11

SINGLE SECTION vs EQUIVALENT 4 SECTION FILTER

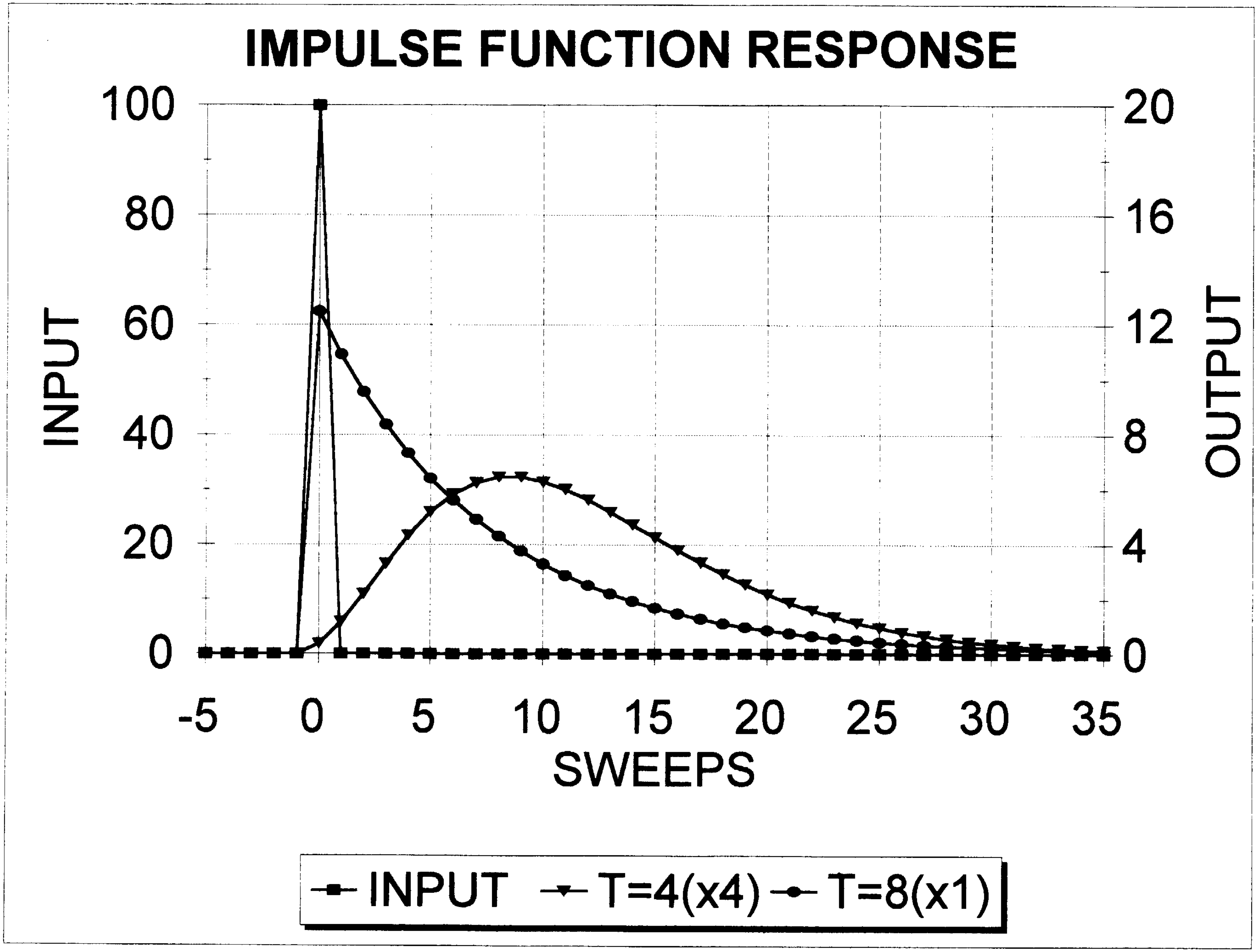


FIGURE No. 12