Building PChem Apparatus

Question: What do I need to learn in order to build a scientific apparatus to solve physical chemistry problem?

In Progress

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Preface to the First Edition

Due to remarkable expansion of technical innovations, now-a-days, many integrated, stand-alone, and ready-to-use apparatus are available to perform routine physical chemistry (abbreviated as PChem in this text book) experiments. It is, however, very advantageous to develop the skills necessary to be able to design and construct an apparatus suitable for a physical chemistry experiment. This "apparatus building"-skill can not only make it easier for one to operate and troubleshoot a stand-alone apparatus, but also offers an opportunity to build an unique (commercially not available) and less expensive (than commercially available) apparatus, which fulfil the demand of ever changing and demanding sophisticated PChem experimental need.

Now-a-days we all recognize the important role of the computer and readily-available computer programs in the design, fabrication, and operation of PChem apparatus. Therefore, the use of computer-assisted drafting, designing, ray-tracing of light and charge particles, and finally computer-aided measurement and automation of PChem apparatus are discussed.

This book is an introduction to data acquisition in physical chemistry for use with any introductory college/university course in analytical chemistry, spectroscopy, instrumentation, or experimental physical chemistry or chemical physics of the kind usually taken by undergraduate and graduate students in science and engineering.

We are writing this book because my experience in teaching undergraduate and PhD students in my own laboratory for last few years has convinced me of a serious need for a book that truly introduces the subject "Building PChem Apparatus" to the college/university science (particularly physical chemistry or chemical physics) students.

We are writing this book with the conviction that any student, even one who has no experience with data acquisition in experimental physical chemistry, should be able to learn what computer aided data-acquisition is, why data acquisition requires special attention, how to use the basic ideas of the subject in designing data acquisition system for laboratory-based experiments, and how different analysis methodologies can be used to organize scientifically important data, while neglecting erroneous ones. I certainly believe that the book can be studied without any help from an expert in the field. The level of mathematics is suitably selected in the book so that any student with basic knowledge of algebra, differentiation and integration would comfortably go through the book.

We sincerely hope that this book will fill in the knowledge-gap and will contribute to the quality and functionality of apparatus built in the PChem laboratories.

A bachelor's degree in chemistry or a related discipline usually is the minimum educational requirement for entry-level chemist jobs. However, many research jobs require a master's degree. Students planning careers as chemists and materials scientists should take courses in science and mathematics, should like working with their hands building scientific apparatus and performing laboratory experiments, and should like computer modeling. Perseverance, curiosity, and the ability to concentrate on detail and to work independently are essential. Because R&D chemists are increasingly expected to work on interdisciplinary teams, some understanding of other disciplines, including business and marketing or economics, is desirable, along with leadership ability and good oral and written communication skills. Graduate students typically specialize in a subfield of chemistry, such as analytical chemistry or polymer chemistry, depending on their interests and the kind of work they wish to do

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Experimental scientist is the profession in which knowledge of the mathematical and natural sciences gained by study, experience, and practice is applied with judgement to develop economically the techniques to discover novel scientific principles for the benefit of overall progress of science.

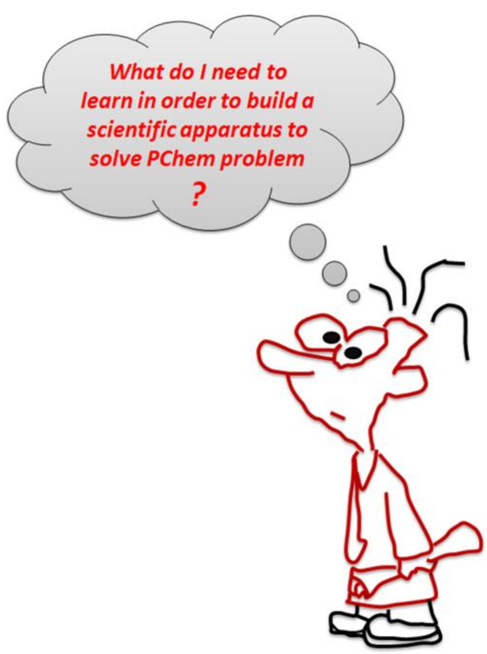
Chapter 1: Introduction

Highlights: What do we need to learn in order to build a scientific apparatus to solve PChem problem?

Like all areas of chemistry, experimental physical chemistry is continually changing, with new discoveries being made all the time. Experimental physical chemists use instruments to observe novel behaviour of atoms and molecules, study intermolecular interactions, prove hitherto-unknown hypothesis in quantum chemistry, optics, thermodynamics, kinetics and catalysis, model combustion reactions and explosives, predict breakdown of pollutants in environment and many other physical or chemical phenomenon. Based on convenience, requirement and specific need, often experimental physical chemists set up, troubleshoot, repair, and construct the instruments they use in measurements. As opposed to a stand-alone system purchased from a commercial supplier, a home-built instrument can have a number of advantages:

(1) Physical chemist can better formulate strategies to test and correct malfunctioning equipment, modify instruments for a particular purpose or construct an instrument which is not commercially available.
(2) A home-built measurement system is always less expensive than a stand-alone system.

However, a number of technical and engineering skills are necessary to construct even a simple model instrument. In this regard, a confused first year PhD student asks the right question:



What do I need to learn in order to build a scientific apparatus to solve PChem problem? This question is relevant when (1) we join an experimental physical chemistry research group (Professors in research institute/university primarily interested in research); (2) we want to join Industry (especially scientific equipment-manufacturing company) after receiving PhD degree (mastering scientific equipment repair/building skill is asset for any employer); (3) we want to join Academia after finishing PhD and post-doctoral works (funding and grants for experimental PChem research are always limited; equipment building/ repair skill/attitude is asset under in fund-constrained research activity).

One quick and easy answer to the above question is perhaps “just get involved in research, you will get to know”. It is indeed a good idea, but only barrier is “Experience”. How do we gain experience? It is often suggested that if PhD work is more focused on science (featuring data interpretation), post-doctoral work must be more focused on instrumentation (featuring scientific equipment building), or the other way around. However, gaining experience through this easily agreeable method, in many instances, does not work just because this mutually complementary opportunity may not be always available in the PhD and Post-doctoral labs. Once an experimental lab is fully functioning, principal investigator tends to solve PChem problems using existing facility (peer pressure and expectation in publishing/patenting works in research university/institute is high). This task requires data interpretation more than instrumentation. As a result, students (both PhD and Post-doctoral) are nudged more into operating the existing facility and into data interpretation.

What is the legitimate solution then? Is it possible to provide some of the initial and essential exposures (of scientific apparatus building skill) through a course/class in PhD curriculum? In principle, answer is yes, it is possible. Is this class/course going to be “another physical chemistry lab” course of the kind usually taken by students in MSc and UG study? Answer is a big “NO”. In general physical chemistry lab course follow “cookbook” style: a fully functioning instrument is provided and students have just operated it once or twice to gather data. Unfortunately, real-life PChem experiments are not “cookbook”. Therefore, the basic philosophy behind the proposed course/class (on Building PChem Apparatus) should be, “Take an instrument which is not functioning at all, make it work, and then take the measurements”. Is it possible to formulate such a course/class? This question takes us to the first question (asked by the confused PhD student):

What do we need to learn in order to build a scientific apparatus to solve physical chemistry problem?

Mechanical Designing ?
Designing of Optics ?
Designing of Charged Particle Optics ?
Designing Vacuum Systems ?
Detectors ?
Signal Transmission ?
Programing ?
Electronics ?
Measurement and Automation ?
Error Analysis ?

Is it a complete list? Legitimately yes, at least we will get an introduction to things that we can learn more thoroughly on our own in future. This systematic initial exposure is expected to make the eventual process easier. This lecture notes will revolve around above-mentioned topics and finally will present designs of the PChem equipments built by renowned scientists and Nobel laureates to solve PChem problems.

Chapter 2: Mechanical Designing and Fabrication

Highlights: Hand Tools, Mechanical Drawing

Introduction:

Data acquisition is a process of measuring electrical signals (generated from physical phenomena, such as temperature rise or pressure drop) from different sensors and transferring.

Hand Tools:

It is highly desired that an experimental PChem student must be familiar with and able to make use of common hand tools to assemble and modify PChem apparatus. It is true even when a PChem student works with instruments that are fabricated and maintained by an operator or a machinist. An elementary knowledge of hand tool operations will allow one to design the apparatus that can be constructed efficiently and at reasonable cost. This section is intended to familiarize the reader with the functions of various mechanical hand tools useful in PChem laboratory. It is always advantageous for PChem scientists to have the entire set of commonly used hand tools available in the laboratory as they are not too expensive and having them around the lab becomes very useful.

While using hand tools it is also desired that a PChem student should adopt a "craftsman like attitude" towards hard tools. This means that an experimental PChem student must avoid making damage to the instrument or its components by using the wrong tools. It is mandatory that an experimental PChem student must be able to make proper use of hand tools. Undoubtedly, this section gives the reader an idea of frequently used hand tools and their proper functions; however, real skill with these tools can be best acquired under the supervision of a competent machinist.

(A) Screw drivers and Wrenches:

Bolt, Nut and Screw:

A bolt is an externally threaded fastener designed for insertion through "clearance hole" in assembled parts and is normally intended to be tightened and released by torqueing a nut. A nut is fastener with a threaded hole. A screw is an externally threaded fastener capable of being inserted into a hole with previously-performed internal thread or with forming its own thread and is intended to be tightened or released by torqueing its head. Figure # gives illustration of bolt, but and screw.

Common tools for driving screws and bolts include screw drivers and wrenches. Usually, a screwdriver is selected as a mating tool for the head of the screw. Therefore, for the election of right screw driver, it is important to be familiarize with common screw heads first.

Figure #: Bolt, Nut, Screw.

Generally, three different sizes (1, 2, and 3) of slotted-head and Phillips-head screw drivers are used. For socket-head screws, allen key or allen drivers are required. Both a fractional/imperial (1/16-1/4 inch) set and a metric (1.5-10 mm) allen key sets are useful because different country uses different set. For an example, if a component is imported from USA, fractional set is required. On the other hand, we mostly use metric set in India.

Figure #: (1) Slotted-head, (2) Phillips-head, (3) Socket-head, (4) Hex-head.

Socket-head and hex-head are frequently encountered in bolds and the most common shape of nuts is hexagonal. Therefore, either open-end or box-end wrenches with both a fractional (3/8-1 inches) and a matric set (10-19 mm) are very useful for hex-head bolts and nuts. Ratcheting socket driver with both fractional (3/4-7/8 inches) and matric (10-19 mm) socket set becomes very handy while working with hex-head bolt and nut. For socket-head bolt and nut, allen key set and right open- and box-end wrenches are required. Adjustable wrenches are also useful while working with bolts and nuts. Here note that pipe wrenches are different from these mechanical wrenches used for bolts and nuts.

(B) Pliers: Pliers are hand tools used to hold objects firmly and to bend and compress a wide range of materials. Some pliers frequently used in PChem lab include combination plier (contain both gripping jaws and cutter, which can be used for gripping, twisting, bending, and cutting), channel-locking plier (this is nothing but adjustable plier), niddle nose plier, diagonal cutter, flush cutter, and forceps.

(C) Hammers: A hammer is a tool that delivers a blow (impact) to an object. Hammers vary in shape, sizes, and structures. A ball-peen hammer (peening means processing surface to improve mechanical property of the metal) is very helpful in PChem laboratory. A soft-faced hammer can also be useful for plastic and rubber inserts.

(D) Files: It is a metal-working tool, with a series of sharp and parallel teeth, used to remove (cut) fine amount of material from the work-piece. Often it is used to rub an uneven metal surface. Files vary in shapes (flat, half-round, and round) and sizes.

(E) Miscellaneous: Scissors.

(F) Electric Hand Tools: In machining, boring is a process of enlarging a hole that has already been drilled. Power hand drill can be used to drill a clearance hole. Note that in PChem labs, we frequently use two types of holes: (1) tapped or threaded holes (2) clearance hole. This comes with different drill bit sizes for boring different holes. **Jigsaw:** to cut arbitrary curves or custom shape in a piece of metal. A power jigsaw is made up of an electric motor and a reciprocating saw blade. Cutting action in reciprocating saw blade is achieved through a push and pull reciprocating motion of the blade.

Data acquisition is a process of measuring electrical signals (generated from physical phenomena, such as temperature rise or pressure drop) from different sensors and

Chapter 3: Working with Vacuum:

Highlights: High Vacuum, Ultrahigh Vacuum, Pressure, Roughing, Turbo Pumps

Why Vacuum in PChem Labs?

A vacuum system produces an environment of reduced pressure which is useful in many physical chemistry experiments. Generation of vacuum may simply be the first step in creating a new gaseous environment (e.g., creation of an inert environment from oxidizing environment). It is necessary to create and sustain vacuum to maintain a clean surface for controlled deposition of atomic or molecular species for catalysis study. In electron- and ion-based spectroscopy and microscopy (e.g., photoelectron spectroscopy and microscopy, mass spectrometry) beams of electrons and ions must be handled in a vacuum (or in vacuo) to prevent loss of momentum through collisions with confounding air particles. Vacuum ultraviolet, extreme ultraviolet, X-ray radiations and far-IR are absorbed by air and thus can propagate over large distance only in a vacuum. Hence, the spectrometers working in these spectral ranges are operated within vacuum containers. To maintain cryogenic (very cold) environment, a vacuum system is an essential part to avoid liquefying air.

Characterization of a Vacuum:

A vacuum environment is primarily characterized by the pressure and the composition of residue gases in the vacuum system.

How to Achieve Vacuum:

Vacuum engineers use different parameters to characterize gas flow. Understanding gas flow (both in molecular and viscus flow regimes) is important to decide pumping speed and nature of the pumps suitable for specific application. Understanding of gas flow also helps design the vacuum line/chamber to achieve desired level of vacuum.

Gas Flow Parameters:

(1) Pumping speed at a point (S): Pumping speed at a point is defined as volume rate of flow through an aperture across a cross-section of a tube. Pumping speed at a point is related to

volumetric flow (not related to mass flow). $S = \frac{dV}{dt}$. **Units are $l\ s^{-1}$, $m^3\ s^{-1}$, $ft^3\ \min^{-1}$, etc.**

The capacity of a vacuum pump is specified by the speed measured at its inlet ($S_P = \frac{dV}{dt}$ at pump inlet).

Pumping Speed (S) is related to volumetric flow (not related to mass flow):
; Nut and Screw:

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Chapter 4: Working with Electrical and Electronic Components:

Highlights: Sensors, Detectors, Relay,

Electrical Safeguard for an Instrument:

A power interruption in the operator's absence threatens serious contamination and damage of the vacuum system both at the time the power goes off and when it comes back on again. When the power goes off, it is essential that the turbo pumps or diffusion pumps stop operating before the fore-line pressure rises about the critical backing pressure. When power is restored in the operator's absence, there is no provision to follow the orderly initiation of pumping discussed before. As a minimum safeguard against a power failure, the power to the system's components should be supplied through power relays that are wired to latch off until reactivated by the operator. A latching relay circuit is shown in Figure #.

Figure # Relay circuit to latch off a pumped high vacuum system.

For a vacuum system that operates for a long periods of time without close supervision, it is worthwhile to incorporate an electrical control system that monitors the pressure in the chamber and the fore-line. Many high quality commercial thermocouple gauge and ionization gauge controllers include relays that can be set to trip at a predetermined pressure. The relay controlled by the fore-line thermocouple gauge can be set to trip at 200 to 300 mTorr. This relay can be wired to operate a second, heavy-duty relay that removes power from the pump. The design of a logical inter-lock system employing temperature and pressure sensors to protect vacuum system will be discussed later.

Data acquisition is a process of measuring electrical signals (generated from physical phenomena, such as temperature rise or pressure drop) from different sensors and transferring

Chapter 5: Working with Charged Particles

Highlights: Sensors, Analog and Digital Signals, Single Ended and Differential Signal Transmission, Signal Conditioning, DAQ devices, LabVIEW

Introduction:

Data acquisition is a process of measuring electrical signals (generated from physical phenomena, such as temperature rise or pressure drop) from different sensors and transferring the signals for storage

Working with Charged Particles (Ions and Electrons)

Chapter 5: PC-Based Data Acquisition

Highlights: Sensors, Analog and Digital Signals, Single Ended and Differential Signal Transmission, Signal Conditioning, DAQ devices, LabVIEW

Introduction:

One of the important skills include the design and fabrication of personal computer (PC)-aided data acquisition system.

It is often stated that 21st century physical chemistry is molecular chemistry and in cutting-edge and state-of-the-art physical chemistry experiments, taking data by hand is not only inconvenient but also quite impossible. With ever-increasing power of PC, automation of data acquisition, analysis, and display from a complete experiment (which can be comprised of one or more physical instruments) can be achieved through PC-based data acquisition system. Realizing the significance of PC-based data acquisition system in physical chemistry measurements, American Chemical Society (ACS) in the guidance of undergraduate education on chemistry stated that laboratory instruction should include practical experience with computerized data acquisition and analysis.{ref: Undergraduate professional education in chemistry; American Chemical Society: Washing, DC, 1999}. The aim of this book is at giving a concise introduction of "PC-based data acquisition" to experimental physical chemistry students.

Over the several decades, National Instruments (NI, USA) has developed LabVIEW (short of **Lab**oratory **V**irtual **I**nstrument **E**ngineering **W**orkbench)-based data acquisition system which is widely adopted as standard practice in industry, academia, and research labs (perhaps include 90% of the market). It is graphically oriented programming language for data acquisition (DAQ) and requires almost no formal knowledge of programming (e.g., C, C++, or Fortran). Experimental physical chemists, who are first chemist by training and profession, and programmer second (they hardly get formal training in programming, particularly in India). In this regard, LabVIEW-based DAQ system can be very useful for physical chemists as it can be implemented very easily and quickly.

Raising Experimental Curiosity:

A few Practical Problems from Physical Chemistry:

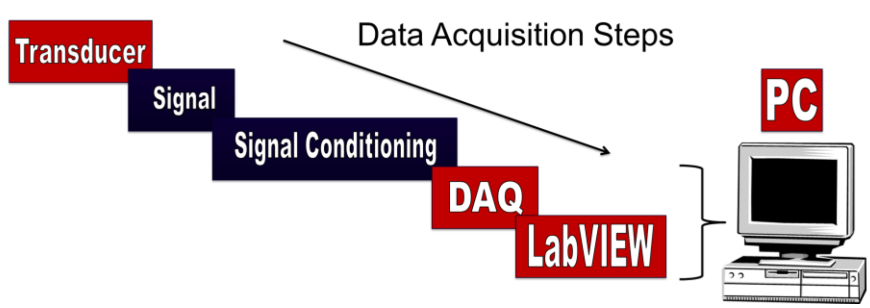
1. Thermodynamics: Heat of reaction (ΔH_r) is defined as the amount of energy or heat absorbed or released in a reaction.

To determine the “”heat of reaction” of a reaction experimentally, we need to monitor the temperature of a reaction over time, using temperature probe (or sensor, e.g., a thermocouple). This experiment is called calorimetry (science of measuring heat). Without a standalone “calorimeter” instrument, how can we perform the measurement and record and plot the data directly in computer hard disk? What are the components required to set-up such measurement?

2. Spectroscopy:

In electronic spectroscopy, we can develop the concept of energy levels (σ, σ^*, π, π^*), interaction of light with molecules, chromophores for $\sigma \rightarrow \sigma^*$ and $\pi \rightarrow \pi^*$ transitions, effect of conjugated double bonds on $\pi \rightarrow \pi^*$ transitions, absorbed color vs. observed color based on the electronic spectra recorded experimentally.#######

Data acquisition is a process of measuring electrical signals (generated from physical phenomena, such as temperature rise or pressure drop) from different sensors and transferring the signals for storage analysis and presentation with a personal computer (PC). Essential components of a generic data acquisition system are schematically depicted in Figure 1. They include: (A) Sensor, (B) DAQ-Device, and (C) Personal Computer (PC). A short introduction to these three elements is given here first. More details of each component will be given later in this chapter.



(A) Sensor: The measurement of a physical phenomenon, such as the temperature of a solution or the intensity of light, begins with a sensor. A sensor is also called a transducer which converts a physical phenomenon into a measurable electrical signal. Depending on the type of a sensor, its electrical output can be a voltage or current that varies continuously with time (a continuously varying signal is called analog signal). Some sensors may require additional components and circuitry (amplifier or attenuator) to properly produce a signal that can accurately and safely be read by a DAQ device. A few examples of sensor include

(1) Thermocouple: used to measure temperature

(2) Photomultiplier Tube (PMT): used to measure or detect photons of light intensity

(3) Multichannel plate (MCP): used to measure or detect ions or electrons (charged particles)

(4) Photodiode: used to measure photon.

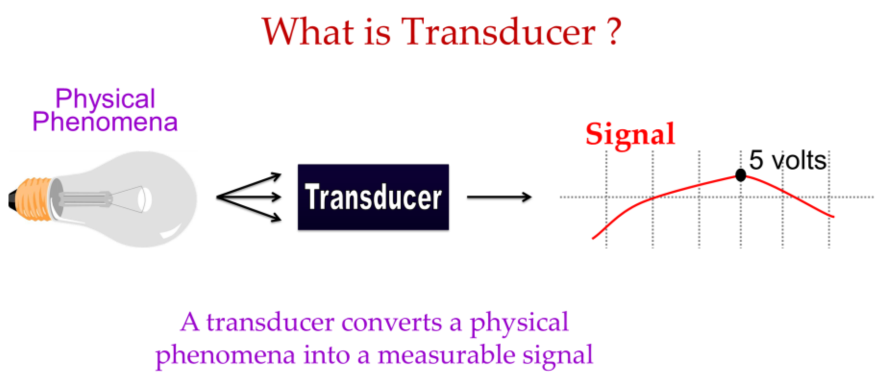


Figure 2: Transducer produces signal from a physical phenomenon

(B) DAQ Device: This interfaces between the computer and sensor. Its primary function as a device is that it digitizes incoming analog signals so that computer can interpret them. Often DAQ devices can perform a variety of functions, such as automating measurement system, digital-to-analog conversion, generation of output analog signal, generation of digital input/output signals, generation of digital pulses as counters. Both "desktop DAQ devices" (such as a plug-in PCI-DAQ board) and "portable DAQ devices" (such as USB DAQ devices) are available from NI.

Analog and Digital Signals:

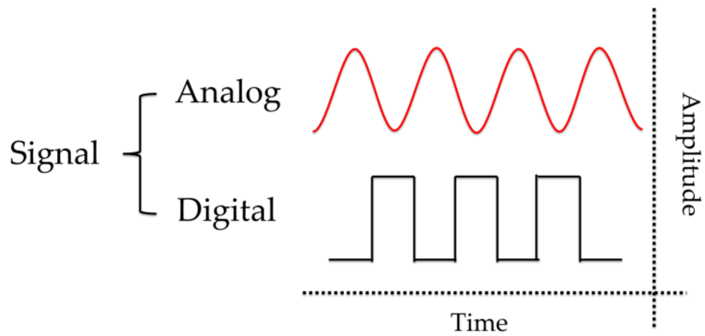
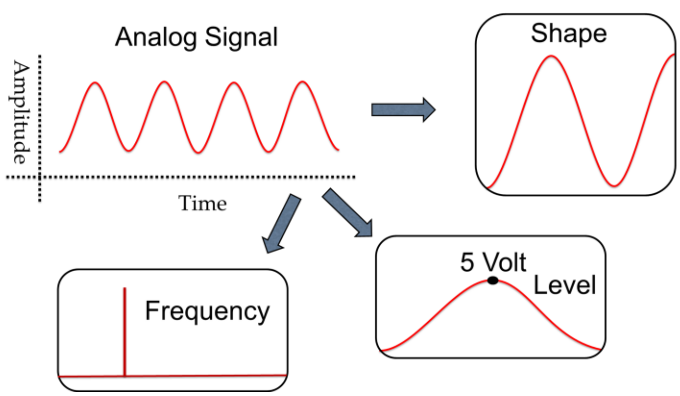


Figure #: Two types of signal: Analog and Digital

Data acquisition begins with the physical/chemical phenomenon to be measured. This physical/chemical phenomenon could be absorption of light by specific molecule (electronic spectroscopy), generation of heat due to endothermic reaction (thermochemistry), or many other things discussed in physical chemistry texts. A sensor or transducer converts this physical phenomenon into a measureable electrical signal, such as voltage or current. Types of signals can be categorized into two groups:

(1) Analog, and (2) Digital.

(1) Analog Signal:



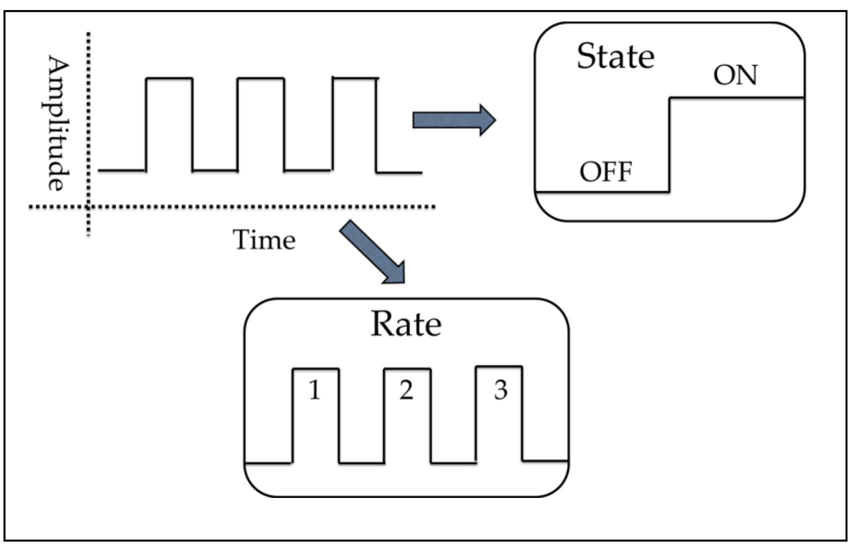
An analog signal is a signal that varies continuously, as depicted in Figure #. In general most of the transducers send analog signals. A transducer transmitting analog signal is also called broadband transducer (sensor). An analog signal can be at any value with respect to time. Bipolar analog signal ranges from a negative to a positive value (e.g., -5 to +5 V). Unipolar analog signal ranges from 0 to a positive value. Any analog signal has three characteristics:

(a) Level, (b) Shape, and (c) frequency;

each contains vital information about the measured analog signal.

(a) Level: The level of an analog signal gives vital information about the intensity of the signal. According to the Figure #, the level of the analog signal is 4.5 volts.
(b) Shape: Analog signals can be identified (categorized) after their specific shape: sine, square or triangular analog signals are depicted in Figure #. One can further analyse the signal based on the shape of the signal (e.g., slope can be estimated).
(c) Frequency: Analog signals can also be identified (or categorized) by their frequency. Unlike level or shape of the signal, frequency cannot be directly measured. The signal must be analysed using the Fourier transform to determine the frequency information.

(2) Digital Signal:



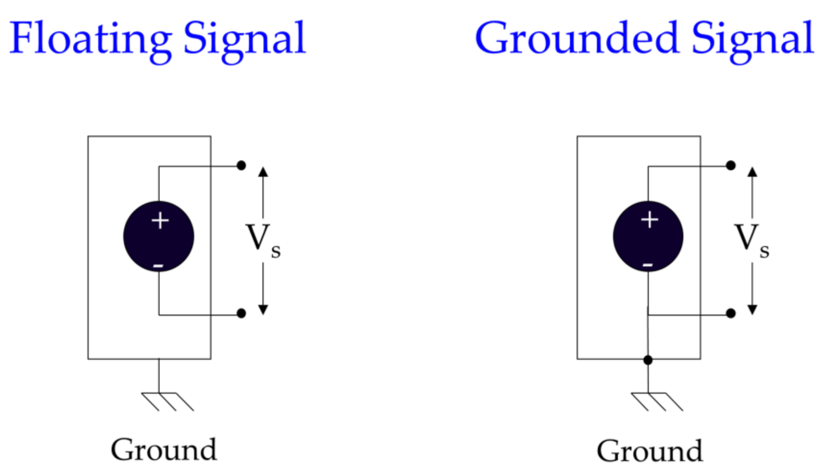
Digital signal cannot take on any value with respect to time; a digital signal two possible levels: high or low. Digital signals are commonly referred to as transistor-transistor logic (TTL) signal. TTL specification features a digital signal to be low when the level falls within 0 to 0.8 V, and the signal is high between 2 – 5 V. Any digital signal has two characteristics:

(a) State, and (b) Rate;

both provides useful information for a digital signal.

(a) State: Digital signal cannot take on any value with respect to time. The state of a digital signal is the level of the signal: on or off.
(b) Rate: The rate of a digital signal defines how the digital signal changes state with respect to time.

Measuring Analog Signals:



To measure analog signals, one must know the signal source: whether (1) grounded or (2) floating? Furthermore, one must also know how the analog signal is transmitted (transmission of signal is called signalling) from the source to DAQ device: whether (1) single ended or (2) differential? Now we shall discuss about “signal source” and “signal transmitting methods”.

- Signal Source:
  (1) Floating signal source: In a floating source the voltage signal is not connected to any absolute reference or common ground. Examples include batteries, thermocouples, isolation amplifier, etc.

(2) Grounded signal source: A grounded source is one in which the voltage signals are referenced to system ground (such as earth or building). The most common examples of grounded signal source include power supplies and signal generator.

If we are using two separate instruments, the grounds of two independently grounded signal sources generally are not at the same potential. The difference in ground potential between two instruments connected to the same building ground system is typically 10 mV to 200 mV. The difference can be higher if power distribution circuits are not properly connected or grounded.

- Signal Transmission:

(1) Single ended: This is the simplest method of transmitting electrical signal over wires. The main advantage of signal ended over differential signalling is that fewer wires are needed to transmit multiple signals. If there are" n" signals, then we need "(n+1)" wires – one for each signal and one for ground. For differential signalling we need at least 2n wires. However, it lacks the ability to reject noise picked up during transmission. This point is explained when differential signalling is discussed.
Examples of single ended signalling include RS232 serial communications, VGA video connector, etc.
When can single-ended signalling be used?
- For signals greater than 1 V.
- For short cable (less than 15 ft)
- For cables travelling through a noise-free environment
- When different signals share a common ground reference

(2) Differential signalling: It is a method of transmitting electrical signal with two complementary signals sent on two paired wires (called a differential pair). Since external noise tend to affect both wires together, and final sampling of the signal is done only by the difference between the wires. This technique is very good at eliminating noise, as depicted in Figure #.
Examples of differential signalling include PCI-express, USB, etc.
When can differential signalling be recommended?
- For low-level signals (less than 1 V)
- For long cable (where there is a high chance of picking up noise)
- When different signals require separate ground-reference
- When cable travels through a noisy environment

Signal Conditioning:

The analog electrical signals generated by the transducer must be optimized for the input range of the DAQ board; e.g., amplifier in which low-level signal should be amplified to increase to increase resolution and reduce noise. Amplifier should be located close to the transducers, sending only high level signals to the personal computer, minimizing the effect of noise on the reading.

Ground in Electrical Connection:

Figure # illustrated a three pin electrical plug. The wire that is connected to ground pin of a plug is connected to the metal body of the equipment. Any leakage current appearing on the metal body of the equipment must be discharged safely to ground so that the user does not get electric shock when using the equipment. The ground pin is made to be longer, so when one inserts the plug, the earth connection is made to the equipment first.

DAQ Hardware:

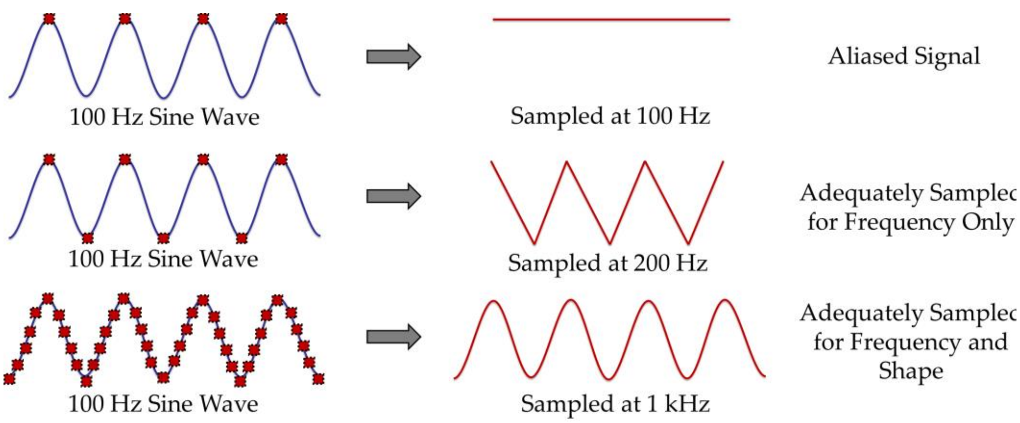
DAQ hardware acts as the interface between the computer and the outside world. The primary purpose of DAQ hardware (device) is to digitize incoming analog signals so that the computer (which is digital electronic device) can interpret them. A DAQ device (hardware) carries out following functions:

(1) Analog-to-digital conversion (ADC)
(2) Digital-to-analog conversion (DAC)
(3) Generating digital input or output (I/O) signals
(4) Counting (events or pulses, etc.)

Based on these functions, most DAQ devices have four standard features: analog input channels, analog output channels, digital I/O, and counters. For an example, NI USB 6008 DAQ device has 8 analog input channels, 2 analog output channels, ….###. NI PCIe 6361 has 16 analog input channels, 2 analog output channels###. While selecting one DAQ device for physical chemistry experiment or measurement, one has to determine these features of a suitable DAQ device based on the equipment and experiment. In the following sections, four standard features will be discussed in details.

(1) Analog-to-digital conversion (ADC): ADC is a process of translating analog signal to digital data so that a computer can process it. This conversion depends on a number of factors:

(a) Sampling Rate: ADC circuit components in DAQ device takes snap-shots of the analog signal (which is continuous in time) and converts into a series of discrete digital (binary) signals at a specified sampling rate. Effect of variation of sampling rate is illustrated in Figure #.



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states that sampling rate must be more than twice the rate of the maximum frequency component we detect to actually represent the frequency of analog signal. Furthermore, sampling rate must be between 5-10 times greater than the maximum frequency component of the analog signal to actually represent the shape of the analog signal.

(2) Resolution: The number of bits that an ADC uses to represent one snapshot of the analog signal is called resolution of the ADC. If a 3-bit ADC is used to sample sine wave analog signal, the digital signal which is obtained after ADC, is depicted in Figure #. A 3-bit ADC divides the full analog signal range into 8 divisions (2^3). Each division represents a binary code between (000) and (111). Figure # clearly suggests that the digital signal does not represent the original signal well and some information is lost in ADC. By increasing the resolution to 16 bits, the number of codes from the ADC increases and extremely accurate digital representation of the analog signal can be achieved.

(3) Range: Range of ADC hardware refers to the minimum and maximum analog signal levels that the ADC can digitize (quantize). In general, it is advisable to pick a range that the analog signal fit in. Smaller range gives a more precise presentation of the analog signal, provided that the signal is not clipped (saturated).

(4) Gain: Gain setting amplifies or attenuates the analog signal for best fit in ADC range. Generally, most DAQ devices offers gain settings 0.5, 1, 2, 5, 10, 20, 50, and 100. Proper

gain setting give more precise representation of the analog signal because this allows one to use all of the available ADC resolution.

Personal Computer (PC):

Different features of a computer used for data acquisition can drastically affect the maximum speed of acquiring data as well as the performance of DAQ system. They include:

(1) Processor Speed: Computer processor is a unit that does the logical operations. Today's technology produces easily investable PCs with processor speed more than 1 GHz (Giga Hertz = 10^9 Hz). This means that the processor can perform one logical operation (e.g., one command) in 10^{-9} second. Ordinary (easily investable) PC can do most of satisfactory DAQ jobs in physical chemistry laboratory with this processor speed. However, additional plug-in processor (e.g., a digital signal processing, DSP, board) may be required for processing very high frequency signal (if data sampling rate is very high).

Processors are also sometimes classified by the number of bits (**b**inary dig**its**, a single bit can take only one of two values: 0 or 1) they can process at one time. A 32-bit processor means that its data registers are 32-bit wide. Larger registers make proessing speed faster. Mostly a 32-bit processor can perform most of the physical chemistry data acquisition jobs. For the application of high frequency data sampling, 64-bit processor can also be suitable.

(2) Memory: Memory, in PC, refers to a physical device that stores data on a temporary basis during data acquisition. It is called random-access-memory (RAM) because data is read and written at the same time. In contrast, in direct-access-memory (e.g., hard disks) the time required to read and write data varies significantly. For data acquisition in physical chemistry problems, more than one Giga-byte (10^9 bytes; where 1 byte = 8 bits) RAM can serve the purpose.

(3) Hard Disk Speed: One limiting factor for acquiring large amounts of data is often the hard disk (direct access memory). High-speed hard-drive (which defines the rate at which data can be acquired and streamed to disk) can speed up data acquisition time and speed. Unfragmented (free) disk space also improves the overall performance of data acquisition system. Speed of reading data in hard disk defines hard disk speed, which is often expressed in terms of RPM.

(4) Communication Buses: Communication bus is a subsystem that transfers data between components inside a computer. It allows us to connect components to the computer processor. PCI slots, USB ports, serial ports (e,g,, RS-232) are commonly used

communication buses in data acquisition system. In general, throughput for a serial communication buses is very limited as compared to parallel communication buses.

(5) Operating System: Choice of selecting an operating system depends on the compatibility with data acquisition devices, registry capacity of the processor, memory, and expertise.

Photomultiplier Tube:

Low-light-level measurement is becoming important in different experimental physical chemistry experiments. This measurement can be done using photomultiplier tube, photodiode, and CCD camera. These detectors convert light into analog electrical signals (current or voltage). However, when light level becomes weak independent incident photons are detected as separate pulses. This is called single photon counting method using photomultiplier tube. This is very effective if the average time intervals between single pulses are sufficiently wider than the time resolution of the photomultiplier tube.

PMT consists of a photocathode, an electron multiplier (composed of several dynodes) and an anode. Photoelectrons are emitted from photocathode. These photoelectrons are multiplied by secondary electron emissions through dynodes and finally collected by the anode as output pulses. In usual applications, these output pulses are not handled as individual pulses but dealt with as an analog current created by a multitude of pulses (analog mode). In this case, a number of photons are incident on the photomultiplier tube per unit time as in Figure # and the resulting photoelectrons are emitted from the photocathode as in @. The photoelectrons are multiplied by the dynodes are then derived from the anode as output pulses as in 3. At this point, when the pulse to pulse interval is narrower than each pulse width or the signal processing circuit is fast enough, the actual out-put pulses overlap each other and eventually can be regarded as electric current with sort noise fluctuations as shown in 4.

In contrast, when the light intensity becomes so low that the incident photons are separated as shown in 5, the out-put pulses obtained from the anode are also discrete as shown in 7. This condition is called a single photoelectron state. The number of output pulses is in directly proportional to the amount of incident light and this pulse counting method advantages in signal-to-noise ratio and stability over the analog mode in which an average of all pulses is made.

INCOMPLETE

Chapter 5: Detectors

Highlights: CCD, MCP, …

Introduction:

We have already seen that modern detectors provide a variety of information on detected physical or chemical phenomenon in the form of pulsed electrical signals. In order to extract this information, however, the pulse electrical signal must be further processed and understood. Pulsed electrical signals are a brief surges of current or voltage in which information (of physical or chemical event) is coded in one or more of its characteristics, for example, its polarity, amplitude, shape, its occurrence in time relative to another pulse, or simply its mere presence. This mode of coding, as opposed to another mode of coding used for continuous signals, for example, amplitude or frequency modulation of a sinusoidal signal,

CCD (charged coupled device):

The charge-coupled device (CCD) is the most efficient device for converting optical image (signal) to electrical signal (they act as optical image sensor). They are very frequently used in video and digital still cameras. This device uses certain amount of electrical charge to represent certain level of light intensity, sampled at discrete times (meaning of discrete time will be addressed soon in this chapter). The CCD image sensors have received great attention because of its superior detection capability and performance characteristics in quantitative imaging systems.

Theory of CCD imaging: A CCD is an integrated circuit etched onto a silicon surface forming light sensitive elements called pixels. Fundamentally, in a CCD image sensor, array of light sensitive cells is used to capture a light image. Each cell is picture element (which is called pixel), as shown in Figure #. Each pixel contains a MOS capacitor.

Capacitor:

A capacitor is an electrical arrangement of conductors and a dielectric medium for string electric charge, like water reservoir for storing up water as shown below.

The acronym MOS stands for metal-oxide-semiconductor. MOS capacitor is made of a metal electrode (often called gate) and a semiconductor. They are separated by insulating oxide oxide dielectric medium. In a CCD pixel the gate (metal electrode) is typically made of heavily doped polycristalline silicon, oxide layer (which can be as thin as 1 nm) is typically made of SiO2 and single crystal silicon is used as semiconductor. In fact, this silicon semiconductor surface also act as support surface for all pixels, which are etched onto this surface as an integrad circuit, as shown in Figure #.

Photons incident on Si surface generate electron-hole pair or free electrons (due to photoelectric effect). Si is a semiconductor with band gap about 1.1 eV (approximately 1000 nm). Therefore, incident light shorter than 1000 nm (1µm) can generate charge (electron-hole pair). The electron-hole pair can recombine and effect of light can be diminished. Under constant illumination, an equilibrium is set up between the rates of incoming flux and charge recombination.

Now amount of charge produced in Si is proportional to the light intensity and that is why in order to measure light intensity quantitatively, we have to measure the electric charge produced by incident light. Figure # illustrates the potential well concept which can be used to quantitatively collect and measure the charge produced by certain light intensity. A thin layer of silicon oxide is grown on a section of silicon surface and a conductive gate is then grown on the SiO2 surface. This composite element is called pixel (picture element). If a positive electrical potential is applied to the gate, electrons generated by the incoming photons are then stored in one pixel. Thus, every pixel acts as potential well in which photogenerated electrons are stored. Each pixel can collect (or store) upto a million electrons.

Here we note that electrons (or charge) can also be generated by thermal agitation (without influence of incoming photons), which is, in turn, stored in pixels. These electrons are indistinguishable from those generated by photon interaction. These electrons are called dark electrons as they are spontaneously generated even in dark due to thermal agitation.

As stated above, a matrix arrangement of oxide and gate structures is fabricated onto a single crystal Si surface (typically 10 cm diameter and 500 micron thickness) so that thousands of potential wells are established across a large area of Si surface. After storing the charges in each pixel, the potential wells are parallelly propagated by application of an appropriate sequence of potential to the gates. This charge transport is illustrated in Figure #, taking an illustrative and oversimplified one dimensional CCD array. Any charge which is been collected at a pixel is carried along the array. This figure illustrates transport of the charge packet from a single pixel. However, in reality, two adjacent wells will have stored charge packets. In CCD sensor, the separation between individual charge packets is maintained during the transfer process and no mixing between wells occurs. Charge packets can be transferred hundreds of times without loss of charges.

Figure # gives an over-simplified version of parallel charge transport concept in CCD sensor. Every vendor has their own proprietary manner of performing this parallel charge transport. Variations between manufacturers can be significant. In many cases, parallel charge transport is not performed at the silicon-silicon dioxide interface; instead, it is performed in a buried epitaxial (made of doped Si) interface (another layer is used between SiO_2 and Si surface). Different manufacturers use different structure of layers to construct pixels in CCD sensors. However, simple concept shown in Figure # illustrates an illustrative example of charge transport used in CCD.

Now one dimensional charge transport concept can be extended to two dimensions. Figure # shows 2D CCD imager. Pixels are always kept square in shape because non-square pixel geometries lead to difficulties in data sampling. Each pixel is capable of storing photoinduced electronic charge. In the illustration (Figure #) each pixel is square (13.5X13.5µm). The two dimensional array of potential well is called parallel register. An image that is focused on the parallel register produces a pattern of charge in proportion to the total integrated flux incident on each photo-site. The serial register, shown at the top of Figure #, is a one dimensional CCD and plays an important role in CCD read-out.

Figure # illustrates the CCD read-out sequence. A programmed sequence of changing gate potentials causes all charge packets stored in the parallel register to be moved in parallel toward the serial register. As a result, the charge stored in the top row is shifted from the parallel register into the serial

Chapter 5: Pulsed Electrical Signal and Its Transmission through BNC Cable

Highlights: Rectangular Pulse, Bandwidth, -3dB, BNC Cable, Characteristic Impedance

Introduction:

We have already seen that modern detectors provide a variety of information on detected physical or chemical phenomenon in the form of pulsed electrical signals. In order to extract this information, however, the pulse electrical signal must be further processed and understood. Pulsed electrical signals are a brief surges of current or voltage in which information (of physical or chemical event) is coded in one or more of its characteristics, for example, its polarity, amplitude, shape, its occurrence in time relative to another pulse, or simply its mere presence. This mode of coding, as opposed to another mode of coding used for continuous signals, for example, amplitude or frequency modulation of a sinusoidal signal, becomes very effective in physical chemistry measurement equipment when detectors are pulsed devices (e.g., photomultiplier tube used in many pulsed laser spectroscopy experiments).

Ideal Electrical Pulse (A Rectangular Pulse) in Time Domain:

To begin the discussion of pulsed electrical signal, let us first identify some basic characteristics of a rectangle electrical pulse, which is encountered frequently. Figure 1 shows an ideal rectangular pulse, either in voltage or current, as a function of time. The pulse duration (defined later in this chapter) of electrical pulse may vary from micro-seconds to fractions of a nanosecond (limited by the response time of modern electronics). Following features are evident.

(a) Baseline:

The baseline of a pulsed signal is the voltage or current to which the pulse decays. This is usually zero; however, it is possible for the baseline to be at some other level due to the superposition of a constant dc voltage or current.

(b) Pulse height or Amplitude:

The amplitude is the height of the pulse as measured from its maximum value to the baseline below this pick.

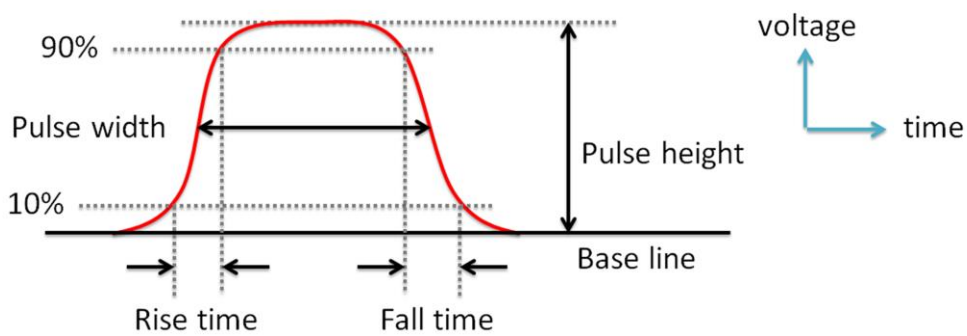


Figure 1: Ideal electrical pulse in time domain. Different features are shown.

(c) Width:

This is the full width of the pulsed signal at the half-maximum of the signal, FWHM.

(d) Leading Edge:

The leading edge is the flank of the signal that comes first in time and the falling edge is the flank which comes last in time.

(e) Rise time:

This is the time it takes for the pulse to rise from 10% to 90% of its full amplitude. The rise time essentially determines the rapidity of the signal and is extremely important for the timing applications.

(f) Fall time:

In analogy with rise time, the fall time is the time it takes for the signal to fall from 90% to 10% of its full amplitude.

(g) Unipolar and bipolar:

A unipolar pulsed signal is one which has one major lobe entirely on one side of the baseline. In contrast, bipolar pulses cross the baseline and form a second major lobe of opposite polarity.

Real Electrical (distorted rectangular) pulse (in time domain):

Thus far, an ideal rectangular electrical pulse signal is presented above. In practice, however, it will be found that rectangular pulses are very often distorted by various factors in the electric circuit. Following figure illustrates a deviated rectangular pulse which is often observed practically.

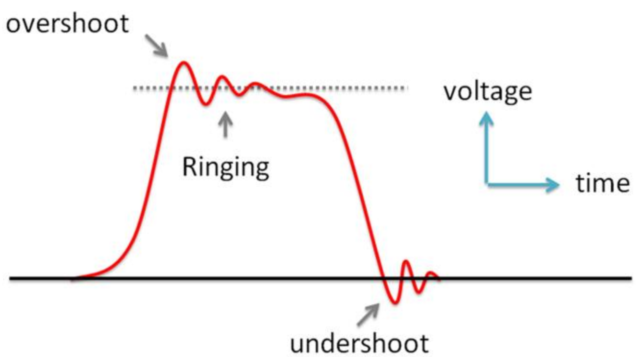
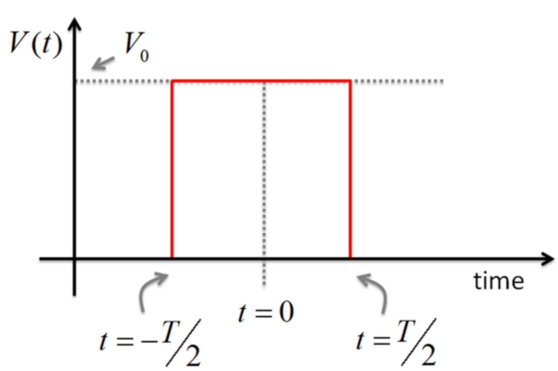


Figure 1: Ideal electrical pulse in time domain. Different features are shown.

The time domain Representation:

Description and visualization of electrical pulses can be easily done in terms of its variation in time. Figure 3, taking an example of voltage variation, depicts square or rectangular pulse by the function $V(t)$, which has an amplitude of V_0, extends from t= -T/2 to t= +T/2 and which is created at t=0. Mathematically $V(t)$ can be represented as follows,

$$\begin{aligned} V(t) &= V_0 \text{ when } |t| \le T/2 \\ &= 0 \text{ when } |t| > T/2 \end{aligned}$$



The Frequency domain Representation:

A pulsed (electrical) signal can be easily visualized and described in time domain; however, a complete understanding of a pulsed electrical signal (especially pulse distortions) also requires viewing (examining) the pulse in terms of its frequency components. From theory of interference in optics, it is well known that a pulse is originated due to a superposition of many pure waves (frequency components). Indeed, if we have a pulse whose shape in time is known, its frequency components can be calculated by using Fourier Transform of the pulse. Frequency spectrum of the pulse can be represented as

$$V(\omega) = \int_{-\infty}^{+\infty} V(t) e^{-i\omega t} dt$$

As a representative example, consider an ideal rectangular pulse of width T, and which is centered at t=0, as shown in Figure 3. Fourier Transform of this function can be written as

$$V(\omega) = \int_{-\infty}^{\lim_{-T/2}} V(t) e^{-i\omega t} dt + \int_{-T/2}^{+T/2} V(t) e^{-i\omega t} dt + \int_{\lim_{+T/2}}^{+\infty} V(t) e^{-i\omega t} dt$$

$$= 0 + \int_{-T/2}^{+T/2} V(t) e^{-i\omega t} dt + 0$$

$$= \int_{-T/2}^{+T/2} A e^{-i\omega t} dt$$

$$= \frac{A}{-i\omega} \left[e^{-i\omega t} \right]_{-T/2}^{+T/2}$$

$$= \frac{A}{i\omega} \left[e^{i\omega T/2} - e^{-i\omega T/2} \right]_{-T/2}^{+T/2}$$

$$= \frac{A}{i\omega} .2i \operatorname{Sin}\left(\frac{\omega T}{2} \right) \text{ [as } e^{i\theta} - e^{-i\theta} = 2i \sin\theta \text{]}$$

$$= \frac{2A}{\omega} .\sin\left(\frac{\omega T}{2} \right) = AT \frac{\sin\left(\frac{\omega T}{2} \right)}{\left(\frac{\omega T}{2} \right)} = AT \operatorname{sinc}\left(\frac{\omega T}{2} \right)$$

The power spectrum which represents the power (intensity) contained in each frequency components is represented as $P(\omega) \sim |V(\omega)|^2$:

$$\text{or, } P(\omega) = (AT)^2 \text{sinc}^2\left(\frac{\omega T}{2}\right).$$

The power spectrum is plotted in Figure 4. It is evident in Figure 4 that, $V(t)$ square pulse contains a continuous spectrum of frequency components from zero to infinity.

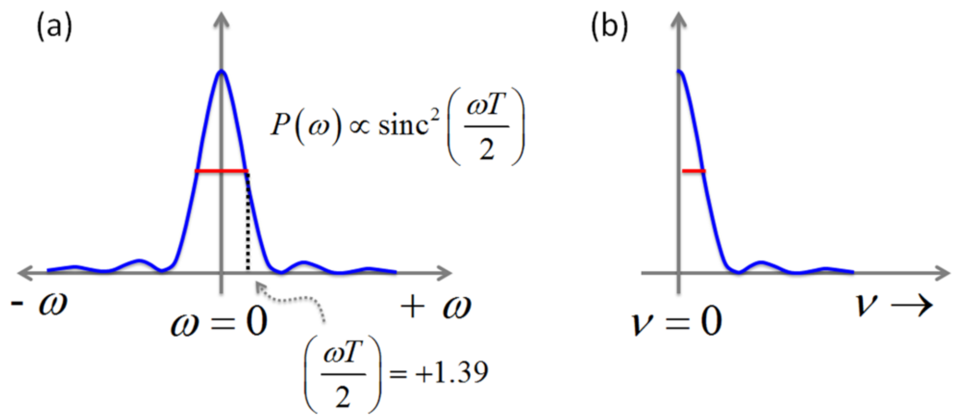


Figure 4:

The amplitude of sinc^2 function decreases by a factor of $\frac{1}{2}$ when $\frac{\omega T}{2} = \pm 1.39$. As the negative frequencies are purely imaginary (mathematical artefact), we can find out FWHM of the real (positive side) power spectrum.

$$\frac{\Delta\omega T}{2} = 1.39$$

$$\Delta\omega T = 2.78$$

$$\Delta\upsilon T = \frac{2.78}{2\pi} = 0.443$$

Thus time-bandwidth product of a square electrical pulse indicates that longer square electrical pulse has a narrow power spectrum and shorter square electrical pulse has a wider power spectrum. This suggests that a rapidly changing signal requires more 'higher frequency' components. Slowly varying signals will contain less high frequency components.

The function $\mathrm{sinc}^2\left(\frac{\omega T}{2}\right)$ spreads out from $\omega = 0$ to $\omega = \infty$. All frequencies play a role in the shaping of the pulse $V(t)$. Thus, in order for an electrical device (for an example, oscilloscope used to visualize electrical signal) to faithfully treat the information contained in the signal, ideally the device must be capable of responding uniformly to an infinite range of frequencies. In any real electrical circuit, undoubtedly, this is impossible. There will be always, resistive components in the circuit, which filters out some frequencies more than others, so that the response is limited to a finite range in ω. This is true even for the interconnecting cables and wires.

The range of frequencies determined by the point in the frequency axis at which the power spectrum falls by $\frac{1}{2}$ of the maximum value is called bandwidth. However, in electronics terminology, the definition of response bandwidth is given in terms of the decibel (dB). The dB is a logarithmic unit of measurement that expresses the magnitude of a physical quantity (e.g., power) relative to a reference level (e.g., maximum value). So, if the frequency component curve is presented in terms of dB $\left[1\,dB = 10 log\left(\frac{P}{P_0}\right)\right]$, we get a response curve presented in Figure 5.

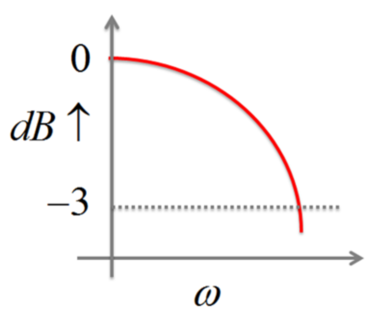


Figure 5.

In the dB scale, power at the half power point (i.e., when power becomes half of its maximum value) is defined by -3dB $(=10\log(0.5))$. Thereby the response spectrum is defined as the range of frequency delimited by the points at which the response falls to -3dB (or by 3dB). This represents the range of accepted frequencies $\Delta\upsilon = \frac{0.443}{T}$ at -3dB power.

In an experiment, when a complete and faithful pulsed signal production is desirable (so that no information from physical or chemical event is lost), electronics have to be selected such a way that the electronic device must be capable of responding uniformly to the bandwidth necessary to represent the electrical pulse (signal). For typical fast pulse of say 5 ns width this would mean that at least $\Delta\upsilon = \frac{0.443}{5\times10^{-9}} = 88.6X10^{+6}$ Hz=88.6 MHz bandwidth is necessary (from zero to 88.6 MHz) to represent the pulse. Therefore, in order to see this pulse in the oscilloscope we need to use > 100 MHz bandwidth oscilloscope.

Furthermore, in general the high frequency components allow the signal to rise sharply, while the lower frequency account for the flat part. Thus, in some experiment if we are interested in fast rising edge of a short pulse, not in the flat parts, eliminating some of the lower frequency does not affect the information in the signal. In most of the physical chemistry experiments which utilize fast electrical pulse to code the information, electronic devices with response bandwidth upto several hundred MHz or 1 GHz are of importance. In the later chapters, we shall see that oscilloscope with response bandwidth in this range will be used to see the optical pulse.

Signal Transmission by Coaxial Cable

"Signal transmission" is guided transmission of a signal (including pulsed) from one part of the electronic device to the other or through the interconnecting cables. A good signal transmission line is expected to preserve the information coded in the signal. In most of the physical chemistry instrumental applications, the standard transmission line is the coaxial cables. These cables are very good for transmitting radio frequency signals (zero to about 10GHz). Here we recall that a pulsed signal consists of a continuous spectrum of frequencies from zero infinity; however, in practice for fast electrical signals (generally, it is on the order of a few nanoseconds), uniform transmission of all frequencies upto several hundred MHz is mandatory to preserve most of the information coded in the pulse. As co-axial cables are very good at transmitting radio-frequency signals from zero to 10GHz, and therefore, are very suitable for pulsed signal transmission. Note that radiation at microwave frequency 3GHz-300 GHz is transmitted in hollow metal pipes called wave guides. In the optical domain, waves can be transmitted by optical fiber.

Co-axial Cable:

The basic geometry of a coaxial transmission line features two concentric cylindrical conductors separated by a dielectric material. A cutaway section of a typical cable showing its construction is depicted in Figure 6. The outer cylinder, which carries the return current, is generally made in the form of wire braid, while the dielectric material is usually polyethylene plastic or teflon, although other material are sometimes used. The entire cable is protected by a plastic outer covering. One advantage of this type of construction is that the outer cylindrical conductor, besides serving as the ground return, also shields the central wire from stray electro-magnetic fields. A variety of cable sizes and designs are available commercially, however, the most commonly used cable is RG-58C/U with 50Ω impedance. 75Ω cable (RG59/U) is also used for high voltage transmission.

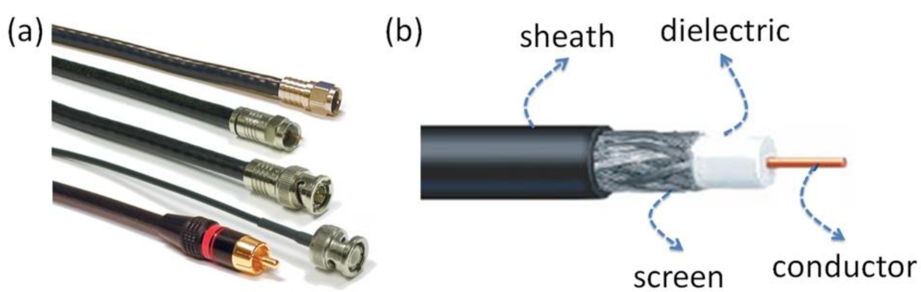


Figure 6:

Signal transmission lines are nothing but conductors. A conductor can store charge which gives birth to magnetic field. Both electric and magnetic fields created by conductor have big consequences on the signal transmission through conductor. Therefore, first we shall review electric filed created by stored charge (this is subjected to Gauss's theorem) and magnetic field created by electric current (this is subjected to Ampere's Circuital theorem).

Gauss's Theorem:

Gauss's theorem is all about finding electric field due to stored charge. Let us assume a positive q+ charge is stored at the center of sphere. Then electric field is directed outward radially (this is the convention). Then at any point outside the sphere (this sphere surface is called Gaussian surface) at a distance r from the center, electric field is expressed as,

$$E * area = \frac{q}{\varepsilon_0}$$

$$\text{Or, } E = \frac{q}{4\pi r^2 \varepsilon_0} \text{ (According to Gauss's theorem.)}$$

This example is a very simple example to demonstrate Gauss's theorem. Actual mathematical form of Gauss's theorem can find total outward flux of an electric field over an enclosed surface.

Gauss's theorem states that the total outward flux equal to the total enclosed charge (called Gaussian surface) divided by the free space permittivity.

The total outward flux of electric field

$$\Phi_E = \oint_s \vec{E}.\vec{ds} = \frac{q_{enclosed}}{\varepsilon_0} \text{ in free space ,} \qquad (= \frac{q}{\varepsilon} \text{ in dielectric medium).}$$

In simple case, if $\vec{E}$ and $\vec{dA}(= dA\hat{n})$ directions are the same and $\vec{E}$ is the same all over the Gaussian surface. $E * area = \frac{q}{\varepsilon}$ (area = total surface area).

This equation states that we can find out electric field due to stored charge over a Gaussian surface.

<u>Idea of Flux</u>:

Let us think of air blowing into a room through a window. How much air comes through the window depends on the speed of the air, the direction of the air blow and the area of the window. The amount of air comes through the window is called air flux. Similarly if there is some charge (e.g., positive charge) stored inside a closed surface, then there will be outward flux of an electric field over his closed surface.

Flux is kind of intensity in terms of particle concept. Field intensity means how many arrows (field lines) are coming.

Electric Field at a point near a charged infinite Conducting wire:

Fig 5

Let us find out electric field at a point near a uniformly charged infinite cylinder (AB) with linear charge density (charge per unit length) $. \lambda = \frac{q_{total}}{L_{total}}$

At a distance r from its axis a point P is taken, where the electric field is to be determined. We need to imagine a cylindrical Gaussian surface of length h through P. Let us assume that wire is positively charged, so that the field $\vec{E}$ at P would be perpendicular to curved Gaussian surface as shown in Figure 5. The flat top and bottom surfaces will have no contribution as the field is tangential to these faces (note that we are interested in knowing outward flux). As all the points P on the Gaussian curved surface (at a distance r) the field will be equal and the total surface is $2\pi rh$

$$2\pi rh * E = \oint_s \vec{E}.\vec{dA} = \frac{\lambda h}{\varepsilon_0} \qquad \text{Or,} \boxed{E = \frac{\lambda}{2\pi r \varepsilon_0}}$$

If the surrounding medium is a dielectric medium then it would be $\boxed{E = \frac{\lambda}{2\pi \varepsilon r}}$.

Ampere's Circuital Theorem:

In Gauss's theorem we have seen that electric field arises due to stored electric charge over a closed surface (Gaussian surface). It is related to the total charge enclosed by the surface. Similarly flow of electric charge (which is known as current) produces a magnetic field (more specifically magnetic flux density, $\vec{B} = \mu_0 \vec{H}$, where μ_0 is vacuum (free space) permeability). Strength of magnetic flux density ($\vec{B}$) can be calculated using Ampere's circuital theorem. It provides a relationship between the magnetic field at a point on a closed curve and the net current through the area bounded by the curve. Mathematically, this means that the line integral of the magnetic field (Induction field $\vec{B}$) around a close path is μ_0 times the total current enclosed by the path. This is similar to Gauss's theorem but one important difference is the integral is over a closed curve (line integral), where Gauss's theorem is based on surface integral.

$$\oint \vec{B}.\vec{dl} = \mu_0 i$$

Ampere's circuital theorem can be best understood by virtue of a long straight conductor carrying a current.

Fig6

Consider a point P at a distance r from the straight, long wire carrying a current i. Due to symmetry the magnetic field $\vec{B}$ at every point on the circle is the same and is directed along the tangent to the circle. According to Ampere's circuital theorem

$$\oint_l \vec{B}.\vec{dl} = \mu_0 i \Rightarrow B * 2\pi r = \mu_0 i$$

Or, $B = \dfrac{\mu_0 i}{2\pi r}$

Self-Capacitance and Self-Inductance:

Fig7

By … ial ca … wo components and how they can be computed by Gauss's theorem and Ampere's circuital theorem.

Self-Capacitance:

In thermodynamics, we have seen that every substance has a certain intake capacity of heat, which is often defined in terms of heat capacity. Heat capacity of a substance is defined as the quantity of heat required to raise the temperature of the substance by 1^0C. In the same way, every conductor of electricity has certain intake capacity of electrical charge (e.g., electrons) which is defined in terms of capacitance. The capacitance of a conductor is defined as the charge required to raise the potential of the conductor by unit volt.

$$C = \frac{Q}{V} = \text{capacitance} \quad (\text{as } Q \propto V)$$

SI unit of capacitance is $\frac{coulomb}{volt}$ or Farad (F). A conductor, thus, exhibits capacitance 1 farad when a charge of 1 coulomb raises its potential by 1 volt.

1F is extremely large capacitance. Generally, practical circuits, including coaxial cables, used in different physical chemistry apparatus, are very small, mostly in the range of microfarads (10^{-6} F) to picofarads (10^{-6} F).

Note: If there is a voltage difference, it means there is an unequal distribution of charge. So conductor has to intake charge to create voltage difference (electromotive force).

A capacitor (also known as condenser) is formed at two electrical terminals (conductors) separated by a dielectric (or insulator), shown in the figure. Coaxial cable exhibits similar configuration in which two concentric cylindrical conductors separated by a dielectric medium, as shown in following figure.

Fig8

Fig9

This configuration is similar to a long cylindrical capacitor.

Let us assume that 'a' is the radius of the inner cylinder, 'b' is the inner radius of the outer cylinder. If the inner cylindrical wire contains λ linear charge density (charge per unit length), then according to Gauss's theorem the electric field ($\vec{E}$) at a distance r from its axis can be expressed as $E(r) = \frac{\lambda}{2\pi r \varepsilon}$ where ε is the permittivity of the dielectric medium.

This is valid for the field close to a long conductor r<<L and $\lambda = \dfrac{Q}{L}$.

Fig10

$$\int_b^a dv = \int_b^a E.dr = -\int_b^a \frac{\lambda}{2\pi r\varepsilon} dr$$
$$(V_a - V_b) = -\frac{\lambda}{2\pi\varepsilon}[\ln r]_b^a$$
$$= -\frac{\lambda}{2\pi\varepsilon}[\ln(a) - \ln(b)]$$
$$\Delta V = \frac{\lambda}{2\pi\varepsilon}\ln(\frac{b}{a})$$

Thus the voltage difference between two cylindrical conductors then can be found by integrating the electric field along the radial line.

(+Ve) charge is in higher potential

This ΔV is the total potential difference between the cylinders A and B.

Then by definition capacitance per unit length (which is called self-capacitance of coaxial cable) will be given as follows.

$$= \frac{\lambda}{\Delta V} = \frac{\lambda 2\pi\varepsilon}{\lambda \ln(\frac{b}{a})} = \frac{2\pi\varepsilon}{\ln(\frac{b}{a})}$$

Here a and b are the radii of the inner cylinder and inner wall of the outer cylinder. ε is the permittivity of the dielectric medium $\varepsilon = k\varepsilon_0$,where k is the dielectric constant. For coaxial cable, typical value of C (self-capacitance) is on the order of 100pF/m.

Self-Inductance:

Like self-capacitance, self-inductance is also a property of the physical arrangement of electrical conductors of coaxial cable. In order to understand self-inductance of a coaxial cable, we shall first review magnetic field created by electric current flowing through a conductor. Apart from permanent magnet, magnetic field can also be produced by electric current through the conductor (this is called electromagnetic field). The magnetic flux (ϕ) through a surface is defined as the surface integral of the normal component of the magnetic induction $\vec{B}$ passing through the surface:

$$\phi_m = \oint_S \vec{B} \bullet \vec{ds}$$

This is a measure of number of $\vec{B}$ field lines are passing through the $\vec{ds}$ surface element. Here $\vec{B} = \mu \vec{H}$, where μ is permeability of the medium and $\vec{H}$ is magnetic field.

Now let us consider coaxial cable. It has two coaxial cylindrical conductors: the outer radius of the inner cylinder is a and the inner radius of the outer cylinder is b. The two coaxial cylinders carry the same current in the opposite directions. Now using Ampere's circuital theorem the magnetic field (more specifically induction field $\vec{B}$) in the dielectric region between the two cylinders at a distance r (the point P) from the axis is, according to Ampere's circuital theorem,

$$\vec{B} = \frac{\mu_0 i}{2\pi r}$$

We note that outside the coaxial cable, the magnetic field is zero as total current enclosed is $(i - i) = 0$. Now we want to calculate total magnetic flux $\phi_B = \oint_S \vec{B} \bullet \vec{ds}$. For this we need to think of the strip of unit length and dr width.

The total area of the strip is $dr \times 1 = dr$. As on this strip $\vec{B}$ is constant and is along the surface normal $\vec{ds}$, we can write

$$\phi_B = B \times (area) = Bdr$$

This is the magnetic field per unit length in the region between the two cylinders at a distance r from the axis. Then total magnetic flux is given by

$$\phi_{total} = \int_a^b Bdr = \frac{\mu_0 i}{2\pi} \int_a^b \frac{dr}{r} = \frac{\mu_0 i}{2\pi} [\ln r]_a^b = \frac{\mu_0 i}{2\pi} \ln\left(\frac{b}{a}\right)$$

Faraday's law of electromagnetic induction states that an electromotive force (EMF) which is nothing by electric potential difference) is produced in a circuit if the magnetic flux is varying with time. When