Notes on Scientific method

What we understand to be Scientific method today is the product of a long evolution encompassing millennia. The development has not been linear, as there are examples of ancients who got it right, but people who came later that were clueless. For instance, Descartes thought that one need only imagine explanations for the natural world around him, and if that did not fit the actual observations, well, that's not his concern. I might point out that Descartes was a mathematician and a philosopher, and philosophers don't require proof of their opinion.

First of all, let's really state what science is all about. Although it has been used to say it's a study of just about anything, more traditionally, it is an effort to understand and predict the natural events that go on in our universe. Initially that universe was really limited to the earth and its natural surroundings. Thus it was called Natural Science. For a long time what people understood from experience, and believed was an explaination for the natural world around them was intertwined with religious beliefs.

Now it is not my intention to give a history lesson, although that would put much of what I have to say in context. Suffice it to say that there is a difference between beliefs which might originate from superstition or religion and the nature of science in its mission to provide understanding. People being human, these are frequently confused. The function of science is to provide a working understanding, and where possible, to predict future outcomes based on this understanding. It is a tool. Science should not be used as a belief, only a working explanation. Thus one should not believe in atoms, the Nernst relationship, the Law of gravitation, or that the sun is in the center of our solar system. All of these things are working explanations that are supported by a huge amount of information, and for which there is no viable alternative. So we use it in the same way we use a wrench. One does not have to believe in a derivative in calculus to use it as a means to determine the slope at a point. Sometime what we think is the total explanation turns out to be part of a much larger explanation. For example, Newtonian mechanics were expanded in the twentieth century with the introduction of quantum mechanics. Quantum mechanics did not prove Newton wrong, only that he was looking at the large scale extremum of quantum mechanics. So in Science, from time to time, we have to adjust the working explanation. Thus it is dangerous to believe that today's explanation and understanding of the universe is dogma. It just might change.

So science is not fundamentally based on belief, but rather of doubt. When one makes an observation, many explanations may be invented to explain it. How does one sort out the many explanations? It is done by doubting them all, and by putting them to the test. And the best test is predictive; that is, if the explanation is true, then it would predict a future observation. Now, what if you start out with a belief, and then look for observations which are consistent with it? In this case, the human mind creates relationships because it wants them to support the belief. This is not science. Science is based on doubt and testing. An example of having the belief prior to observation and disregarding testing that might undermine it is Creationism. Because it is not based on doubt, by definition Creationism is not science, but it is certainly a belief. It would be a mistake to think that this is the only example, and numerous scientists in the past, and even some in recent times have fallen into the same trap. It is the human condition to want to believe in things. In the 90's, and with very little data to support it, a few scientists claimed they had cold fusion. They wanted to believe that they did. Fortunately, so long as political and religious forces stay out, science is self correcting; the forces of doubt came into action, and the claim has been put to rest, though not surprisingly, there are a few who still believe that it exists.

I want to say a few words about two fundamental concepts: Induction and deduction. Many books have been written on both topics, and I can't possibly do any of them justice here, but they are both very pertinent to scientific method. Succinctly, Induction is the process of making observations and deriving a theory or working explanation from them. Deduction involves using a theory to predict outcomes. Newton worked inductively when he used Kepler's planetary data and derived a mathematical relationship describing planetary motion. Deduction is most frequently used by students when they employ an established relationship, as for instance a Name Reaction. When the chemist gets to the bench, and the name reaction does not quite give the expected results, the chemist must use inductive reasoning in order modify conditions to achieve those results. Science which breaks new ground always uses a combination of deduction and induction, as the old is always the foundation for the new.

Which brings us to scientific method itself. Remember that science seeks to create an understanding of our world. The first step is always an observation. The observation will die if the observer does not have both curiosity and creativity, for it requires our observer, our hero scientist, to be interested in that observation, and to go further to propose a basis or explanation for that observation. This is the formulation of an hypothesis, kind of a test theory. The observer ought to base the explanation first on what he or she already understands and may be pertinent. In other words, formulate the initial hypothesis on deduction. *The observation must lead to the proposal of the hypothesis, not the other way around. Remember you are not doing science if you already have an explanation and you are looking for observations to justify it.* You will naturally distort the meaning of the observation to suite what you believe.

And now the good scientist attempts to kill the explanation by subjecting it to doubt, and by testing it. Under ideal conditions, one prefers to use it predictively, but often circumstances prohibit this. One should be very suspect of hypotheses which are capable of limited testing. For instance, offered explanations of events prior to the Big Bang. Hypotheses which fail to predict correctly new observations must either be modified or discarded. In science it is typical that a substantial amount of iteration occurs between hypothesis, testing, failure, modification, further testing, etc. This world between observation, hypothesis and testing is where most of us live.

Let's look at an example of proper formulation of an hypothesis. Let's say that we drop bromine into an unknown substance, and the mixture loses its color (observation). We know that certain types of functionality react with bromine to discolor it (deduction). We can propose that the unknown contains one of these functionalities. We test that hypothesis by using an alternate analysis that would correspond to detecting one of the proposed functionalities, say ^{13}C NMR. A pair of peaks in the right region would support our hypothesis that there is a double bond. Let's say that no such peaks are found in the ^{13}C NMR corresponding to any known functionality that reacts with bromine. Our data shows that the unknown does react with bromine, however. From our data, we can now induce a new hypothesis that what we have is a new example of a functionality that reacts with bromine to discolor it. How do we test this reformulated hypothesis? First, we characterize the compound independently to identify what functionality it does have. Then we characterize the products of the reaction with bromine. Now we test the hypothesis (let's assume one functionality in the molecule) that this reacts with bromine. Part of this process is to check the literature for prior examples of this functionality reacting with bromine. Next we deliberately create a well-characterized example of a compound with the functionality and test it with bromine. If it reacts as proposed, the hypothesis is supported. If it fails to do so, we have to go back and see what was overlooked and formulate a new hypothesis. It is important to understand that in testing an hypothesis, all of the test results have to be accounted for. You are not allowed to cherry-pick only those results that support your hypothesis. This is where many of the religion-based hypotheses fail.

Let's look at the wrong way to formulate a hypothesis. Let's say our hypothesis is that genetically modified foods are harmful. First, the litmus test: did observation lead us to propose this hypothesis, or was this a position already believed that we are looking to support? If you look into the popular press, the latter you will find to be true, thus it would be an unsupported hypothesis. These are the hypotheses that Sherlock Holmes warned us about, as they will lead you to invalid conclusions. Suppose for a moment that an observation was made that a person did in fact become ill after consuming genetically modified food. We can now make a supported hypothesis that there may be a correlation between genetically modified food and illness. It is now up to the researcher to prove this hypothesis WRONG by using every test he can imagine. Only if the hypothesis survives the onslaught of every effort to disprove it, that we can accept it as apparently true. So far, all assays fail to support this hypothesis.

Now, what do you do if your testing gives mixed results? Some testing supports your hypothesis and others do not. Let's say our hypothesis is that the reaction of an acid chloride with an amine gives an amide, a hypothesis we formed when we observed that acetyl chloride and methyl amine formed methyl acetamide. When we go to test this we find that methyl amine and dimethylamine form amides, but trimethylamine does not. Was our original hypothesis completely wrong? No. Was it as widely applicable as we initially thought? Also no. So we must modify our hypothesis to say that Acyl chlorides and amines bearing a hydrogen on the nitrogen form amides. We can now go on to test that hypothesis.

Part of testing a hypothesis is use of the literature. Although by and large you can use the results of others, you must always keep in mind that their results are in context. In other words, it is entirely (and often frequently!) possible that their reported results only occur if what they did to get them is reproduced EXACTLY. Not everyone keeps a sufficiently detailed notebook, and it is not unusual for someone to incorrectly rely on a poor memory when writing up. Thus you should use the literature to guide you, but if there is one report that stands against all of your results, you need to reproduce the published results for yourself. You should not accept it as is. You are now testing their hypothesis. By this means Science corrects itself. It does happen that people publish incorrect conclusions. It is perfectly kosher for you to test someone else's hypothesis and report a different result.

Where the hypothesis survives repetitive testing and becomes generally accepted in the scientific community, it becomes a Theory. In modern times greater theories are rarely the accomplishment of a single person, but by an orchestration of the results of many. Woodward and Hoffman assembled their famous rules as an overarching Theory on the extensive results of many hundreds of researchers who came before them. Keep in mind that some new later evidence may require modification of the theory, so even a theory is not set in stone. Exceptions to Woodward-Hoffman rules have been found. Chemical bond theory has been evolving for the last two hundred years, and quantum mechanics was hardly the last word on it as people made new molecules that bent and twisted bonds. The wall of great theories is composed of the bricks of lesser theories. Most of us contribute our bricks of lesser theories in our own research by publishing. A few lucky and insightful of us will assemble those bricks into a wall. Thus we have atomic theory, the theory of relativity, bonding theory, and a host of others.

There is something beyond a Theory. It is a Law. In the past, a few intrepid souls have had the audacity to unilaterally proclaim a theory with no known exceptions and name it a Law. This is done by personal *fiat*. Thus we have the Law of Gravity, the Laws of Thermodynamics and others. By rights, there should be a Law of Evolution, but all the Laws were created in the 19^{th} century or before, and there is no man of sufficient stature in this century to proclaim such a law. Thus Evolution will forever remain a Theory.

This concludes my comments on Scientific method.