RESEARCH IS ENGINEERING

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What follows is an imaginary dialogue that embodies the elements of many real conversations I have had with students. The two participants are SI SORP (Student In Search Of a Research Project) and PI NORA (Professor In Need Of a Research Assistant).

SI: I hear you might have an opening in your group for a student ready to do thesis research in chemical engineering.

PI: Right. Would you be interested?

SI: It depends. I've heard that you work with molecular beams but I really don't know what they are or what they're good for.

PI: Well, you might say that what we do is like playing billiards. We shoot individual molecules at surfaces or other molecules in a vacuum and see how they bounce.

SI: I don't understand. It doesn't sound like chemical engineering to me.

PI: Let me explain. Do you know anything about cyclotrons and other kinds of accelerators that physicists use, sometimes called atom smashers in the popular press?

SI: I've heard about them and read some articles in magazines and newspapers.

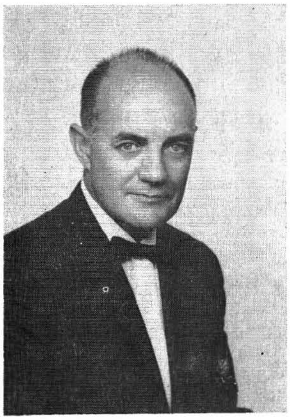
PI: Have you ever seen pictures of particle tracks in an emulsion, or a cloud chamber or a bubble chamber?

SI: Yes, but I haven't thought that much about what they mean.

PI: Look at it this way. Suppose you put a billiard ball on a table and hit it with the cue ball. What would happen?

SI: The billiard ball would go in one direction and the cue ball in another. The particular directions and speeds would depend upon how hard and how head-on the collision was.

PI: Right. Now suppose you replaced the billiard ball with an egg.



John Fenn received his B.A. from Berea College (1937) and his Ph.D. from Yale (1940). After a number of years spent in private industry he went to Princeton in 1952 and remained there until joining the chemical engineering department at Yale in 1967. He has been visiting professor at the University of Trento, Italy, University of Tokyo and Australian National University. He recently received a Senior Scientist Award from the Alexander von Humboldt Foundation in West Germany. He is the author of "Engines, Energy and Entropy: A Thermodynamics Primer."

SI: Well, the same thing would happen, except that the egg's trajectory might be different because it isn't spherically symmetric like a billiard ball. If the cue ball were going fast enough the egg would break and splatter. Also, the cue ball wouldn't change direction quite as much.

PI: Suppose the egg were hard boiled.

SI: Then about the same thing would happen, except that the cue ball would have to be going faster to break the egg. And the result wouldn't be as messy.

PI: In other words, you could tell the difference between a billiard ball, a fresh egg, and a hard boiled egg by observing the trajectories of the cue ball and its target before and after collision. Indeed, you could learn something about their structure and behavior.

SI: I see what you mean.

PI: Well, that's what so-called scattering or collision experiments are all about. The tracks in photographic emulsions and cloud or bubble chambers that you've seen pictures of are trajectory traces, usually of one of the collision partners and the fragments after collision. Essentially, all our knowledge of nuclear structure and reactions has come from the study of such particle tracks.

SI: Very interesting . . . but I don't want to be a nuclear physicist.

PI: Wait a minute. Nobody said anything about your becoming a nuclear scientist or engineer. Using an egg as an example of a target didn't mean that I thought you might want to raise chickens or make omelets! I was just pointing out that what happens when objects collide can give information on their structure and properties.

SI: OK, but I still don't see any connection with chemical engineering.

PI: Let's look further. What are chemical engineers concerned with?

SI: Let me see. Well . . . you know, making plastics, fertilizers and pharmaceuticals, refining petroleum, processing foodstuffs . . . things like that.

PI: Quite a variety, right? Now what do most or all of these activities have in common?

SI: I guess you could say they all involve some sort of chemical reaction. Then, too, there is usually heating and cooling and mixing and distillation and . . . fluid flow . . . and . . .

PI: Good. You've just been reciting what chemical engineers once considered the basic building blocks of their discipline, the so-called **unit operations.** Actually, that term usually referred to physical phenomena like vaporization, crystallization, fluid flow, heat transfer, adsorption and so forth. Chemical reactions were similarly classified in such categories as oxidation, reduction, alkylation, polymerization, hydrolysis, and the like, that were known as **unit processes.** But we can pursue this reduction to fundamentals even further. If you stop to think, you will realize that all of these unit operations and processes are based on the transport of mass, momentum and energy and the transformation of composition by chemical reaction.

SI: I see what you're driving at. The next thing you will tell me is that all of these transport and reaction processes depend upon what happens when molecules encounter each other.

PI: Exactly. You can go to the head of the class. When we scatter a beam of molecules by another beam or a static cloud of molecules, and watch how they bounce, that is to say, what happens to their trajectories, we obtain information on their structure and the nature of the forces between them. The difference between what we do and what atom-smashing physicists do is largely a matter of energy. Physicists are concerned with forces that hold the nucleus together and that relate to energies of billions of electron volts. Chemists are concerned with extranuclear phenomena involving forces which bind electrons to the nucleus and hold molecules together. Chemical energies are always less than a few tens of electron volts. Incidentally, an electron volt per particle (atom or molecule) is equivalent to about 23 kcal/mol. Thus, we don't need and cannot use the billion volt beam energies that the nuclear physicists require and that make their accelerators so big and expensive. By the same token, we cannot see individual collision events as they can. A particle travelling with energies in the millions or billions of electron volts can go through a photographic emulsion or a bubble chamber as if it weren't there. The energy required to make its track is a negligible fraction of the total. On the other hand, an atom or molecule with only a few electron volts of energy won't even make a dent in an emulsion, let alone a track through it. Consequently, molecular beam scattering experiments of the kind we do depend upon bringing about as many collisions as possible that are as nearly identical as possible. Each collision contributes a little bit to the observed signal, usually an electric current obtained by converting the beam molecules into ions.

SI: All right. I can see how such experiments might tell us about the structure of atoms and molecules, but we already have that information about practically all species the chemical engineers are concerned with.

PI: That's quite true, but there is another difference between atom smashing and molecular beam scattering experiments. Consider reactive scattering events that change the composition or structure of at least one collision partner and are the primary interest of nuclear physicists. The energy which seems to count in bringing about nuclear reactions is translational kinetic energy. At least that is the only kind of energy that physicists have a handle on. Chemists, on the other hand, have long recognized that molecules can have several kinds of energy: translational, vibrational, and rotational energy, as well as electronic excitation energy. Most classical gas phase reactions experiments measure composition change with time in a container of reactants at a uniform temperature that can be varied from experiment to experiment. Unfortunately, rotational, vibrational, and translational energies all change with temperature. Consequently, it is generally impossible to isolate the effects of these different forms of energy on the rate or mechanism of the reaction. Indeed, a molecular beam experiment 20 years ago was one of the first bits of tangible evidence that translational energy was not a very important component of activation energy in some reactions. Since then, of course, hindsight and laser experiments have everybody convinced that vibrational energy is much more important in many, if not most, reactions involving reactants with more than one atom.

SI: Are you saying that excited state intermediates are not important in nuclear reactions?

PI: I guess that's what I am implying, but I should retreat a bit because I am not expert in nuclear affairs. It does seem that physicists can't control internal (nuclear) energy states of colliding partners as readily as chemists can control vibrational and electronic excitation. Consequently, the role of excited internal states in nuclear reactions is not as clear as it is becoming in chemical reactions. But there is still another difference in kind between atom smashing and molecular beam scattering experiments.

SI: What is that?

PI: We have been talking so far about reactive scattering. There are two other kinds of collisions that are more important to chemists and chemical engineers than to nuclear physicists. **Elastic** collisions are those in which both momentum and translational kinetic energy are conserved but there is no change in the structure or internal energy state of either collision partner. Then there are **inelastic** collisions in which there is no change in structure but there is a change in the vibrational, rotational or electronic energy of one or both partners. The trajectories of the participants in these kinds of collisions generally respond less to intra- than to inter-molecular forces that are generally repulsive when molecules are close together, attractive when they are further apart. It is convenient to characterize these forces in terms of the work required to pull the molecules apart to an infinite separation, i.e., where the forces are zero. A plot of this work as a function of intermolecular separation is called an intermolecular potential because the work required for separation is equivalent to a potential energy.

SI: Oh, I'm beginning to remember. Didn't we discuss something in our transport course called a Lennard-Jones potential which governs the interaction between two molecules?

PI: That's right. The Lennard-Jones or 12-6 potential model assumes the actual potential is a simple sum of repulsive and attractive potential energies that are inversely proportional respectively to the 12th and 6th powers of the distance between the molecules. The difference between these two powers leads to net repulsion when the molecules are close together and net attraction when they are far apart. Real potentials are more complicated and cannot be accurately described in terms of only two parameters. For many engineering approximations, a Lennard-Jones model is sufficiently accurate to be useful. Which leads me to a question. Why did the subject of potentials come up in your transport class?

SI: We were learning about the dependence of viscosity, thermal conductivity and diffusion in gases upon the forces between molecules! In fact, don't I remember that it is possible to determine the parameters of a potential from measured values of the transport properties and the equation of state?

PI: Correct. But there is a problem. These macroscopic properties represent the integrated or average result of collisions taking place over a wide range of energies, orientations and impact parameters (a measure of the head-on-ness of a collision). For any particular property and set of conditions, there are many combinations of potential parameters that will match a computation with a given experiment. Consequently, it is hard to choose the best one. Moreover, one cannot be sure that a particular potential which matches computation and experiment over a particular range of conditions will give reliable results outside of that range. In addition, it frequently turns out that a potential that works for one transport property, e.g., thermal conductivity, gives unreal results when used to calculate another transport property, e.g., diffusion coefficients.

SI: So what's different about potentials obtained from scattering experiments?

PI: Such experiments probe the intermolecular potential much more directly and with greater sensitivity than macroscopic property measurements. The net result is that potentials based on scattering experiments are more accurate, particularly at separation distances where attractive forces are important. Note that if one does the arithmetic correctly a calculation based on a particular potential can lead to only one possible value of a transport property for a particular temperature and pressure. The converse is not true. There are many possible potential parameter combinations which can lead to a given value of transport property.

SI: I'll take your word for that but it sounds more like science than engineering. Why should engineers do molecular beam scattering experiments?

PI: To answer that question I guess I need to know what you think engineers should do.

SI: I believe engineers should be concerned with practical problems. At least they should try to solve problems in a practical and efficient way. More than that, I guess I believe that they should work on problems that have some commercial impact or significance. If an engineer needs to know the viscosity and thermal conductivity of a gas to design a heat exchanger he can look them up in a handbook or measure them directly. All this business about molecular beams, scattering experiments and intermolecular potentials sounds like pretty esoteric science to me. Maybe it's all right for chemists, but chemical engineers? . . . . I dunno.

PI: I understand your reaction. You say engineers should be practical and efficient. If you need the value for a property like viscosity, "you could look it up" as Casey Stengel used to say. If a value isn't available then you could measure just what you need, but you wouldn't bother measuring what you don't see an immediate need for.

SI: Right on.

PI: Let's look at the heat exchanger problem a little further. Suppose an engineer is trying to design one as a preheater for a cracker but that the client isn't exactly sure what feedstock he will be using. Depending on the time of year and the market it may vary from a mixture of ethane and propane to a melange of several alkanes. In fact, suppose the client's specification calls for a design which can accommodate any arbitrary mixture of 30 hydrocarbons from C_1 to C_8. To simplify the problem for our purpose let's suppose that the mixtures would be binary. There are 450 possible combinations if we include like pairs, i.e., the case of a single species feedstock. Now let's assume that temperatures range from 300 K to 700 K and that the concentration of one component in the other can be anywhere from 0 to 100 per cent. If we further assume that it would take measurements at 10 concentrations to cover any unlike pair and at 10 temperatures to cover the range we're talking about, something like 42,000 data points would be needed to map the entire temperature composition surface for any one property. If it took an average of only one hour for each point, two solid years would be required for the measurements. Of course, by judicious choices and by taking advantage of behavior similarities one could cut down substantially on the actual number of measurements required, but to obtain enough data would still be a formidable undertaking.

SI: I agree, but how would scattering measurements be any better?

PI: As you might guess my choice of problem here was not entirely whimsical. A few years ago a student in my lab determined total cross-sections for the scattering of an argon beam by those 30 hydrocarbons. From these cross-sections she was able to obtain the so-called C_6 values, the coefficients of the r^{-6} attractive term in the Lennard-Jones potential. She found that the coefficient of the r^{-12} repulsive term could be estimated from condensed phase densities, values for which are available. Then she made enough scattering cross-section measurements of one hydrocarbon on another to satisfy herself (and me) that the so-called geometric mean mixing rule was effective enough to give reliable C_6 values for any hydrocarbon pair from the argon-hydrocarbon result. We haven't checked it out yet but we are reasonably confident that similar estimates can be made for the C_{12} coefficients of the r^{-12} term. In sum, from 30 measurements which took about two weeks after the machine was set up, we were able to get 450 C_6 values. Let's allow another six weeks to get estimates for C_{12} and to do a little cross-checking. We would then have a Lennard-Jones potential for all possible hydrocarbon pairs. A computer could be programmed to handle this information and presto!—we can in principle get a printout of all transport properties at any temperature for any binary or multicomponent mixture of these hydrocarbons. I submit that this "esoteric science" is engineering at its best—practical and efficient!

SI: I'm impressed! But still, somehow that kind of research seems more like science than engineering. I'm not quite comfortable with the prospect of a thesis on molecular beams.

PI: OK. We'll come back to that problem in a minute. But first let me make another point about molecular beam research. Did you know that there are a number of articles and processes of commerce based on molecular beam technology?

SI: Is that a fact? Tell me more.

PI: To begin with there is the atomic clock. Until 1967 the standard unit of time, the second, was defined as $(31{,}556{,}925.9747)^{-1}$ of the tropical year 1900! Since then it has been officially defined as the "duration of 9,192,631,770 periods of the radiation corresponding to the transition between two hyperfine levels of the fundamental state of the atom of cesium 133." The device that provides a signal of the corresponding frequency to an accuracy of one part in 10^{11} or 10^{12} is a molecular beam apparatus that one can buy off the shelf. Thus any laboratory can have a primary time standard for not a whole lot more than a very fine Swiss watch! Much less than an astronomical telescope and computer. Then there are lasers, the direct descendants of the maser that was first embodied in a molecular beam experiment. You may remember reading in the papers a few years ago about the uranium enrichment plant which West Germany had agreed to build for Brazil. Political pressure from the U. S. delayed the project but I understand it is now moving again. That plant was based on the so-called "trennduse" or separating nozzle process that stemmed directly from university research in Germany on the same kinds of molecular beam systems we use in our laboratory. One of the hottest high technologies in thin film-solid state electronics is called "molecular beam epitaxy" which permits the growth of single-crystal-like films of very precisely controlled semiconductor compositions on appropriate substrates. The method allows *in situ* synthesis of complex compounds in layers whose thickness is measured in Ångstroms. At last count there were fifty or more companies and institutional laboratories developing this art and five companies engaged in manufacturing the equipment for it.

SI: Golly! Molecular beams are getting to be big business, aren't they?

PI: Yes, but that is neither the only nor the best reason for chemical engineering students to engage in molecular beam research. Let's go back to what you said a few minutes ago, that molecular beam research was more like science than engineering. You've mentioned some of the things engineers do. Let me hear how you define "engineering." What do you think are its essential features?

SI: I guess I would say that engineering is the design, construction and operation of structures, plants and processes that produce useful goods or perform useful services.

PI: Not bad. But what do you mean by "useful?"

SI: Hmm. I guess to be considered useful in the sense I am thinking about something would have to have commercial or market value. Of course, an activity can be useful because it is informative or constitutes an exercise for somebody's talents, but I think it would have to result in actual or forseeable market value to qualify as engineering. If the result were only interesting but non-marketable then I guess I would call the activity science.

PI: Well, that is a conventional point of view, and very thoughtfully put, by the way, but it troubles me. Suppose somebody designed and built a microwave antenna dish as part of a relay station in a long distance communication network. That would qualify as engineering by your definition, wouldn't it?

SI: Of course.

PI: Now suppose that same person designed and built a similar antenna for use in radio astronomy simply to listen in on the stars. Would he be an engineer? Not according to your definition, I think. You would say he was a scientist.

SI: That's a tough call.

PI: Let me try you again. A former classmate of mine designed and built a reactor which comprises a 100,000 gallon tank. The reaction medium is perchlorethylene, dry cleaning fluid. The product is volatile and at very low concentration in the medium. To recover it, a recycling stream of inert gas is bubbled through the tank and passed through an adsorbent that captures the product selectively. Would the design, construction, and operation of this system qualify as chemical engineering?

SI: I would certainly say so.

PI: OK. Now let me tell you that the product is a radioactive isotope of argon which is formed in extremely low yield when a neutrino flux passes through chlorine-containing material. The rate of formation in the tank is of the order of 5 to 10 atoms of argon per day! The whole purpose of the enterprise is to measure the neutrino flux from the sun. Is it still chemical engineering by your definition?

SI: I think I've painted myself into a corner. My instinct tells me that in view of its objective that project should be called science. Logically, I must admit that it sure looks like engineering.

PI: Why can't it be both?

SI: What do you mean?

PI: I think that a lot of semantic confusion arises when we try to classify activities in terms of why people do things rather than in terms of what they do. To me, engineering is the art of applying quantitative knowledge to the solution of various kinds of problems. It is really irrelevant whether the objective is to make a salable product or to obtain a publishable bit of information.

SI: You mean it's what a person does rather than why he does it that counts?

PI: Exactly. Especially from the standpoint of what kind of education and training he gets. Take farming for example. A poor man farms for money. He tries to make a living. A rich man often farms with money. He wants to lose money. That is, at least on paper so that he can claim a tax deduction. They both practice agriculture. My wife loves flower gardening and does it for purely aesthetic and recreational returns. She also is practicing agriculture. Three people with entirely different motivations all practicing the same kind of art.

SI: You mean that there is no difference between science and engineering?

PI: What I mean is that they are not mutually exclusive categories. An activity should not be considered as either science or engineering. In fact, engineering is an art that scientists practice. It is an art that people other than scientists also practice. In other words, all scientists are engineers but not all engineers are scientists. Such an assertion would offend many scientists and more engineers but I think it is true.

SI: I'll have to think about that one.

PI: The important point is that engineering is an art; "the systematic application of knowledge and skill to achieve a desired result." In addition, an engineer must make educated guesses or hypotheses about what he doesn't know and put everything together in the design of a gadget, an experiment or a computer program aimed at achieving his objective. He then makes tests, modifies his design in light of test results, makes further tests and continues this iteration until his objective is realized within his limits of tolerance.

SI: That sounds reasonable.

PI: There's another point to be made. As in the case of any other art, engineering must be learned by practice. Like playing tennis, composing music, or painting pictures, it can't be taught in the classroom or learned from a book. The needed knowledge and the rules can be learned from books or in classrooms, but not the art of using them. That must be practiced, preferably under the guidance and supervision of a master practitioner. Medical schools are well aware of this truth and acquaint their students with the "factory", *i.e.,* the hospital and clinic, early in their professional education experience. Later they serve an apprenticeship as interns and residents during which they practice the art of applying what they have learned, in association with and under the guidance of accomplished experts.

SI: I'd never thought of physicians and surgeons as engineers, but I see your analogy.

PI: In a sense medical schools do a better job of engineering education than most engineering schools. Unfortunately, to provide the same kind of practical experience for its professional students a chemical engineering department would have to operate, or participate in the operation of, a chemical plant or an oil refinery. That just isn't feasible in a university. What a university can do, is expected to do and be in the forefront of, is research. Research consists in learning all that is already known about some aspect of a subject, making guesses about what isn't known, designing an experiment or program based on this knowledge and the guesses, performing the experiment and then evaluating the result from the perspective of previous knowledge and the judgment of peers and experts. In my view that process of scientific research embodies the very essence of engineering and is the most valuable part of an engineering graduate educational experience. It doesn't really make much difference what is chosen as the particular topic or objective. The important point is that the student, on his own but with expert guidance, undertakes and completes a project which involves these important components: 1) learning what is already known; 2) making guesses or approximations about what isn't known but is necessary for: 3) the design of an approach or program or experiment; 4) execution of the program or experiment; 5) exercise of judgment in the evaluation of the result. In sum: Research *is* Engineering.

SI: That's a provocative statement!

PI: Yes, I guess it is and I know there are a lot of my industrial brothers who would take issue with it. They say that universities are ivory towers where researchers are out of touch with reality, that they don't have to face up to real world constraints like budgets, materials limitations, personnel problems, and competition. I have

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type of chemical engineer; one capable of assimilating the imported technologies and of developing new processes more suitable to the efficient utilization of our resources. This requirement provides one of the fundamentals for curriculum development; the other is a sound knowledge of what chemical engineering is.

With these two points in mind, we propose the formation of an "Academic Commission" on a national level, composed of highly qualified professors from all parts of the country who would coordinate the design of a curriculum which could then be implemented at all government sponsored schools. This curriculum should contain a fundamental core of basic science (chemistry, physics and mathematics), with strong interaction through practice in lab sessions. The second stage of the curriculum should emphasize the fundamentals of chemical engineering (thermodynamics, transport phenomena and reaction engineering). Finally, the third stage should be flexible and concentrate on several aspects, depending on the region of the country or the strength of the faculty at hand. As examples, important areas to cover are process design and development, project engineering, energy resources, and equipment design.

It is obvious that the implementation of the proposed curriculum requires highly trained teachers and researchers. These people should be educated through the graduate programs now existing in Mexico; therefore, those programs should be strengthened and strongly supported at the main government sponsored institutions. Furthermore, since all these programs offer only a M.S. degree thus far, emphasis should be placed on the development of one or two doctorate programs at the schools with the capabilities to implement them. Clearly, UNAM is one of them.

Strengthening the graduate programs should also develop research in chemical engineering, which so far has been meager and is greatly needed for the development of our industry. The few people that are presently capable of doing this have been schooled abroad. We feel that we have reached the stage where it is possible, and in fact imperative, to do it in Mexico. □

BOOK REVIEW: Optimization

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ance, just the *how* for a few cases. The *why* is needed so the student can develop, understand and use other designs. It is surprising that the Newton-Bairstow method for curve fitting is not given.

Chapter 3. This chapter, though well-written, desperately needs more worked examples. On p. 102, the concepts of consistency and efficiency should be included with unbiasedness as properties of an estimator.

Chapter 4. This chapter appears to be a literature search from a thesis. The notation will be confusing to older readers whose formal mathematical background predate 1955 but who apply mathematics daily. A glossary of symbols would help. The coverage is excellent in scope. The section on interval reduction is very good. It is unfortunate that the Kuhn-Tucker conditions for constrained optimization are not mentioned. The basis for several algorithms are described but no executable algorithm is actually given. Completed examples are rare; *no* student exercises are provided. There is no warning against sectioning.

Chapter 5. This is an improvement over Chapter 4 in that stepwise algorithms are given but not worked.

Chapter 6 contains only four complete examples to illustrate applications to physical processes.

Chapter 7 is descriptive in nature. For the two "examples" of simulation models, only the results were given. □

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spent about half as much time in industry as in academic institutions and I can tell you that the neurial, competitive and cost conscious as anything in the "real" world. Our budgets are even more inflexible than those of our industrial brothers. We can't pass cost overruns on to our clients, customers, or stockholders, for example. I suggest that when you hear someone say that research in academe is not the real world, you are listening to a person who doesn't know what he's talking about, who is so unaware of the actualities of university research that his own perspective is unreal.

SI: Well, you have certainly given me some food for thought. Let me digest it for awhile and come back to see you again.

PI: Fine. When you come I'll take you through the lab. It may make you feel better. It has 500-gallon tanks, 32-inch vacuum pumps, 6-inch valves and piping, and 10-horsepower motors. You'll think you're in a factory! □