

AN OPEN-ENDED PROBLEM IN CHEMICAL REACTION ENGINEERING

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THE HOMEWORK AND examination problems that students encounter in a traditional chemical engineering class typically have unique correct solutions. Such problems certainly provide necessary practice in applying the fundamental course concepts, but if they are used exclusively students might believe, improperly, that all engineering problems are similarly structured. Worse yet, an exclusive diet of well-defined, single-right-answer problems might leave students unprepared for the more open-ended problems they will face in industry or in graduate research. While it is true that students are generally exposed to a measure of open-ended problem solving in the capstone design course, such exposure is comparatively brief and it occurs late in the curriculum.

Recognizing the importance of open-ended problems in engineering and their under-representation in the traditional engineering curriculum, the chemical engineering department at the University of Michigan set a departmental goal of increasing our undergraduates' ability to solve open-ended problems. To achieve this goal we assign at least one open-ended problem in each of our required undergraduate classes. The structure of the open-ended problems is such that they are major, semester-long projects in which students work together in groups of three to five. The open-ended problems offer natural opportunities for

the students to develop problem-solving and life-long learning skills, to think creatively and innovatively, and to exercise engineering judgment.

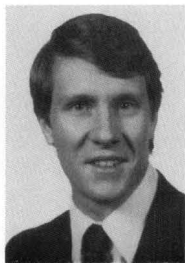
This paper describes my experience in implementing an open-ended problem in our junior-level chemical reaction engineering class. The problem, which involves evaluating and designing a reactor for destroying organic compounds in an aqueous waste stream, is one that could be easily and profitably used at other universities.

PROBLEM DESCRIPTION

The open-ended problem placed the students in the chemical reaction engineering group of a multinational chemical processing corporation. Their company generated aqueous waste streams that needed to be treated before being discharged into the environment. Incineration was presently being used. On December 7, 1988, the CEO of the company read a short article in the *New York Times* (Figure 1) about an alternative method of treating wastewater streams that involved reacting the organic constituents with oxygen at elevated temperatures and pressures. He wanted to know if this technology, termed wet oxidation, was something his company should be using. After trickling down through a few levels of management, the assignment eventually reached the reaction engineering group (*i.e.*, the students). The groups' stated mission was to evaluate the wet-oxidation technology, make a recommendation about its technical feasibility, and finally, to size a reactor (or process) and specify its operating conditions.

The students received no information other than the scenario above and a copy of the *New York Times* article. There were no restrictions on their use of outside sources of information (*e.g.*, the library, industry, government agencies, personal contacts, *etc.*) so progress down this avenue was limited only by their imagination and initiative. Another available pathway to information was their corporation's Technical Service

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This paper describes my experience in implementing an open-ended problem in our junior-level chemical reaction engineering class. [It] involves evaluating and designing a reactor for destroying organic compounds in an aqueous waste stream, . . . [and] could be easily and profitably used at other universities.

THE NEW YORK TIMES, WEDNESDAY, DECEMBER 7, 1988

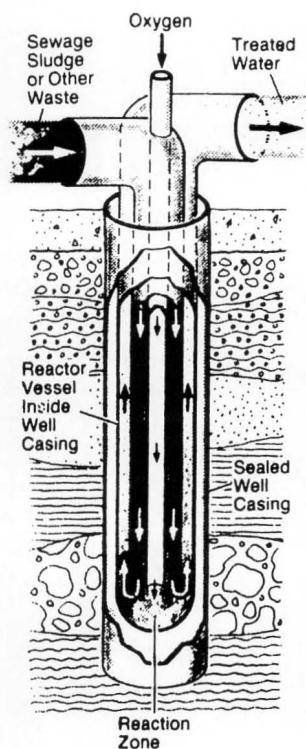
Treating Waste 5,000 Feet Down

If a wet waste material, like sewage sludge, is mixed with oxygen and placed under high pressure, it undergoes a process that chemists call wet oxidation. The sludge, whose disposal is becoming a burden to more and more municipal sewage plants, is converted to relatively clean water and sterile ash.

Such processes, when carried out on the earth's surface, require elaborate vessels under high pressure, special pumps and ample acreage for buildings and equipment. But a Dallas company, the Oxidyne Group Inc., has developed a system that moves the process to the bottom of a well 5,000 feet underground, where it is carried out in a sealed reactor vessel.

In the process, sludge is pumped to the bottom of the well. Because of the weight of the sludge coming down the pipe, pressures at the bottom of the well can exceed 2,000 pounds per square inch. Oxygen is sent down through another pipe and the wet oxidation begins.

Raw sludge is constantly pumped into the system and treated water and ash come out. Wet oxidation produces considerable heat, some of which can be used to drive the process.



SPECIFICATIONS
About 5,000 feet
2,000 psi
550 degrees Fahrenheit

hazardous waste problem. Rather, the goal was to develop an open-ended problem in chemical reaction engineering of sufficient complexity to challenge the students without simultaneously overwhelming them.

THE SOLUTION PROCESS

Background Information

The students' initial activity involved gathering information about wet oxidation in general, and the Oxidyne process mentioned in the *New York Times* article in particular. Several groups called or wrote to Oxidyne to learn more about their process technology and its applicability to their particular waste stream. Other groups resorted to the library in search of background information on wet oxidation and vertical, underground wet oxidation reactors. Although the literature provides limited descriptions of underground oxidation reactors [1,2], it is rich in general descriptions of wet oxidation processes [3-8]. Of course, the presence of this information in the literature did not mean that the students, who apparently had little training in performing literature searches, would find it. Indeed, very few groups were adept at locating the relevant papers and patents.

The Search for Data

All of the groups realized that they needed much more data than they initially received in the problem statement. In memos to the Technical Service Director, they requested essential data such as the flow rate, density, temperature, and composition of the aqueous waste stream and the concentrations of the various components. I played the role of the Technical Services Director, but this assignment could also be delegated to a teaching assistant if desired. For this problem, I specified a wastewater stream at ambient temperature flowing at 30 liters/minute. The stream contained 1% each of phenol, chlorophenol, and acetic acid. The precise composition of the stream is, of course, arbitrary, but it is for these three compounds that the literature [5, 9-14] provides the most kinetics data for the wet oxidation reactions. One perceptive group realized that the component concentrations in a real process could exhibit fluctuations even though the process was nominally at a steady state. They sent a memo asking whether such variations occurred and if so, what their magnitude was. To avoid introducing

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FIGURE 1

Department. This department would conduct *experimental* work for them, but the students had to define clearly the precise experiments they wanted done and the data they desired to be reported. Additionally, the Technical Services Department conducted experiments only in response to written memos directed to the Technical Services Director.

Note that the scenario described above was not intended to represent the way a real corporation operates. Likewise, the data used in this problem (presented in the next section) were not necessarily intended to mimic those associated with a genuine

unnecessary complexity into the problem I told them that the variations in concentration were sufficiently small that they could be safely neglected.

Another piece of information that the students needed was the maximum permissible concentrations of the organics in the reactor effluent. Different groups took different approaches to obtaining this information. Nearly every group did some library research in an attempt to find environmentally acceptable discharge levels for phenol, chlorophenol, and acetic acid. Most groups, however, found an apparent lack of readily available, specific guidelines. Some groups contacted the State of Michigan Department of Natural Resources for state regulations, others contacted the EPA for Federal regulations, still other groups contacted environmental engineers in local industries (*i.e.*, Dow Chemical), and one group contacted the Ann Arbor Waste Water Treatment Plant. Through these and similar efforts the students were able to select reasonable effluent concentrations for the three organic constituents of interest in this problem.

At this point, reaction rate data for the wet oxidation of phenol, chlorophenol, and acetic acid were the only missing pieces of information. Interestingly, only one group recognized that the library was a rich source of reaction rate data, and this group, after a thorough literature search on wet oxidation, was able to obtain sufficient literature data to proceed with the reactor design. In fact, this group was so intent on tracking down all possible literature sources that when they found a reference to a MS thesis on oxidation in supercritical water [14] they contacted the University of California at Berkeley, where the research was conducted, to obtain the author's current address and phone number so that they could consult with him and obtain a copy of his thesis. The members of this group were rewarded for their independence and for realizing that the library, and not the laboratory, is the first place to look for kinetics data.

The other 19 groups relied on the Technical Services Department as their primary source of kinetics data. These groups submitted memos outlining the experimental conditions to be used and the data to be taken. With very few exceptions, the groups' first attempts at identifying conditions that would produce useful rate data were unsuccessful. They typically selected initial reactant concentrations that were too high to allow for isothermal operation of a laboratory reactor (the wet-oxidation reaction is very exothermic) or combinations of temperature and residence time that led to very high conversions at very short times (oxidation reactions are very rapid at elevated temperatures). An additional problem that some

groups encountered was that they requested data that were not as useful as they had envisioned. For example, one group requested that the Technical Services Department run a wet oxidation reaction in an isothermal CSTR, sample the liquid phase at specified times, and identify and determine the concentrations of the different components. They were planning to use the concentration vs. time data to derive the reaction rate laws. Of course, concentrations do not change with time in a steady-state CSTR; thus the reply memo from the Technical Services Director showed that the component concentrations in the effluent stream, though lower than those in the feed stream, remained time invariant. Upon examining the reply memo, the group eventually realized its mistake. The next memo requested experiments in a batch reactor wherein concentrations do change with time.

The groups' requests for reaction rate data, expectedly, covered a wide range of temperatures, pressures, and initial concentrations. To accommodate each request precisely would have been impossible without extensive laboratory work. Thus, when a group identified experimental conditions that could lead to the acquisition of useful kinetics data, my reply memo consisted of a handout containing much of the literature data available for the wet oxidation of phenol [5, 9-12], chlorophenol [5, 11-13], and acetic acid [14], the three compounds of interest in this problem. The experimental conditions under which these data were taken covered temperatures from 185 to 445° C, pressures from 54 to 240 atm, and initial reactant concentrations from about 50 to 12,000 ppm. It included data obtained from both batch and plug-flow laboratory reactors.

Because the data given to the students were real experimental data taken directly from the literature, they reflected experimental uncertainties, and they contained occasional bad points. Furthermore, because I used different data sets taken by different investigators under different experimental conditions and interpreted using different assumptions, the collection of data given to the students was not entirely internally consistent. Thus, in interpreting their kinetics data and deriving reaction rate laws, the students had to exercise judgment and decide which data sets were the most reliable for their design calculations.

Reactor Configurations and Operating Conditions

Having obtained all the necessary flow rates, compositions, and kinetics data, the students next began to consider the issues involved in selecting and designing a wet-oxidation reactor. Because the *New York Times* article described a vertical oxidation reactor

that descends 5,000 feet below the surface of the earth, all of the student groups took this reactor configuration as their starting point. Most groups began trying to model such a reactor using a combination of ideal reactors. Several groups contacted Oxidyne for more information about their reactor systems and for assistance in their modeling efforts. These initial modeling activities revealed that the students perceived their assignment to be sizing a vertical, underground oxidation reactor. By unnecessarily confining themselves to a specific reactor configuration so early in the solution process, however, they failed to see the broader issues involved in the problem. Therefore, I spent a few minutes of class time encouraging them to think about the real problem (which was not necessarily the same as the stated problem) in which the CEO was interested. After some discussion along these lines the students began to realize that the real problem was not simply to size an underground oxidation reactor, but rather for their company to make its products without experiencing any adverse environmental consequences. Upon identifying the real problem, many groups began to develop ideas such as modifying the manufacturing process to minimize the amount of waste produced, developing new technologies that generated less or more easily treated wastes, separating and recovering the components in the waste stream, and exploring alternate means of wastewater treatment (*e.g.*, ozonation, biodegradation, and the use of catalysts). Not all groups explored all these themes, of course, but all of them did at least broaden their scope from the initially narrow one that considered only the underground reactor.

After examining several alternative solutions to the real problem, many groups concluded that because the wastewater stream flow rate was low, and because it was relatively dilute there were no real advantages in using an underground reactor. These groups then proceeded to design a conventional above-ground reactor suitable for wet oxidation. They used either a PFR or a CSTR as the basis for their design calculations.

The majority of the groups, however, decided that an underground oxidation reactor remained as the best possible solution. These groups sent memos to the Technical Services Director requesting, among other things, the location of the chemical plant that generated the wastes, the composition of the earth's crust at the plant site, the thermal diffusivity of the ground, and the population density around the site. I tried to keep the problem general and also minimize the amount of data I had to manufacture by replying

that because the corporation was multinational it sought a technology that could be implemented anywhere in the inhabited world.

Most groups demonstrated a reluctance to deviate from the operating conditions of 2000 psi and 550°F (288°C) noted in the *New York Times* article, and their final designs typically specified conditions near those. Although the students realized that reaction rates increased with temperature, they seemed quite hesitant to specify higher reactor temperatures. Interestingly, a few groups thought that the critical temperature of water, which is 374°C, posed some sort of thermodynamic barrier that dare not be crossed during the reaction. These groups carefully designed their reactors so as not to exceed this critical temperature.

After some discussion . . . the students began to realize that the real problem was not simply to size an underground oxidation reactor, but rather for their company to make its products without experiencing any adverse environmental consequences.

The origin of this mistaken impression is unclear, especially considering that the students were given experimental rate data taken at supercritical conditions [13,14]. Several groups, fortunately, realized that the critical temperature was not a barrier, and they selected high temperatures that led to high reaction rates. These groups, through reading the literature [1,13-17], came to appreciate the unique advantages that supercritical operation offers.

SUMMARY OF STUDENT SOLUTIONS

The fact that the assigned problem was truly open-ended in the sense that multiple solutions existed was verified by the diversity in final designs. Of the twenty groups working on the problem, eleven selected underground oxidation reactors such as the one described in the *New York Times* article. Eight groups decided that the underground reactor afforded few advantages for this particular application, and they selected a more conventional above-ground flow reactor (*e.g.*, PFR or CSTR). One group apparently found the decision of reactor placement a difficult one, so these students designed a reactor that they claimed could be operated either horizontally above the ground or vertically underground to meet the plant manager's preference. It is interesting to note that the majority of the groups retained the vertical, underground design and the operating conditions highlighted in the brief *New York Times* article. I think it is unlikely that any of these groups would have recom-

mended such a reactor configuration had they not first read the newspaper clipping. Thus, in this case, the final solution tended to reflect the initial information given to the students.

The final reactor designs also exhibited tremendous variety in their mode of operation (e.g., isothermal, adiabatic, and non-adiabatic reactors with heat transfer were all recommended) and operating temperatures (170 - 727°C). The calculated reactor volumes varied by six orders of magnitude as the smallest reactor volume was 0.845 liters (roughly the size of a pop bottle) and the largest was 494,000 liters (roughly the size of three large railroad tank cars). The fact that different groups arrived at very different final designs can be attributed primarily to the different interpretations of the experimental kinetics data, the different operating conditions and reactors selected, and the different effluent concentrations deemed to be acceptable.

SKILLS USED AND DEVELOPED

This open-ended problem gave the students an opportunity to use and develop several different types of skills. Indeed, a thorough solution to the problem required the students to exercise their technical, problem-solving, and communication skills.

• **Technical Skills** *Technical skills were developed via the students' application of some of the key concepts of chemical reaction engineering. Topics such as modeling ideal reactors, obtaining and analyzing experimental rate data, performing energy balances for an exothermic reaction, handling situations with multiple reactions, and dealing with transport effects in gas-liquid reaction systems were all components of the open-ended problem solution. Several of the groups also wrote computer programs to solve the simultaneous mole and energy balances that arise in this design problem.*

• **Problem-Solving Skills** *In addition to practicing the application of course-specific technical topics, the students also exercised more generic problem-solving skills. For example, they gained an appreciation for the importance of problem identification and definition. The exercise in distinguishing between the real problem and the apparent problem, which incidentally is unique to open-ended problems, helped the students to generate alternative solutions to the one initially identified by the CEO. This open-ended problem also forced the students to adopt and develop a problem solving strategy. They had to identify the important issues involved in the problem, plan a means of addressing those issues, and plan an experimental program (or literature search) for obtaining the required data. The problem also allowed the students to be creative, innovative, and resourceful. Most of the students enjoyed this aspect of the problem for they rarely have this freedom when solving more traditional homework exercises. Furthermore, through this open-ended problem, the students gained an appreciation for the issues involved in solving a complex problem. They realized that a completely rigorous approach to the design of a wet-*

oxidation reactor for a multicomponent mixture was beyond their level of knowledge and beyond the scope of the course. Thus, the students had to decide where they could make assumptions that would simplify the problem without seriously compromising the final solution. Not all groups were equally adept at this task, however, and several groups seemed perfectly comfortable making assumptions that simplified the problem but did not reflect reality. One final skill that this problem afforded the students was the opportunity to sharpen their engineering judgement. The groups had to decide what type of reactor to use, what operating conditions to select, whether or not to use an underground reactor, and how to analyze their ambiguous reaction rate data.

• **Communication Skills** *The structure of this semester-long open-ended problem was such that it included a large amount, and different types, of writing. For instance, the students wrote one-page memos to the Technical Services Director when they needed experimental data. They also submitted a two-page (maximum) progress report around the middle of the semester, and then a comprehensive final report at the end of the semester. This emphasis on technical writing was intentional. In fact, portions of two different class lectures were devoted to a discussion of the key elements of good technical writing, and the students also had an in-class exercise wherein they revised a poorly written paragraph taken from one of their peers progress reports. To provide the students with an additional resource, I also used *The Elements of Style* by Strunk and White as a required text for the course.*

I encouraged the students to write each memo and report thoughtfully by returning for revision any written document that contained more than three grammatical or stylistic errors (e.g., sentence fragments, lack of subject-verb agreement, excessive use of passive voice, etc.). As expected, revisions were frequent early in the semester. I wanted the students to learn from their mistakes, however, and not necessarily be punished for them. Therefore, revising a memo did not affect the student's grade, but merely delayed their receipt of experimental results from the Technical Services Department. A revision of the progress report likewise carried no penalty other than the extra work associated with turning in the report a second time. Revision of the final report, however, did lead to a ten percent reduction in the group's score for the project. Only four of the twenty groups had to revise their final reports, however, and even those four reports showed signs of having been written carefully and thoughtfully.

SUMMARY AND RECOMMENDATIONS

The open-ended problem described in this paper provided a good opportunity for the students to apply key elements of chemical reaction engineering in addition to developing more generic problem solving skills and communication skills. Most of the students enjoyed the problem and the departure it presented from the more conventional homework exercises.

One point that resonated from the student evaluations at the end of the semester was that the course, as a whole, involved too much work. I recognized that this open-ended problem would require a significant effort from the students, so I covered one less chapter

in the text than I had previously covered in the course. Apparently, however, the omission of this one chapter did not compensate for the addition of the open-ended problem. Therefore, care must be taken to ensure that the incorporation of a major open-ended problem is accompanied by the reduction of other assignments so that the students are not overloaded. Fortunately, the open-ended problem described in this paper is sufficiently flexible that it can be modified to suit an instructor's preferences and the time available in the course. For instance, the amount of student effort required can be reduced by providing literature data [5, 9-14] for the kinetics, specifying the desired concentration of organics in the effluent, or specifying a single organic pollutant in the wastewater stream rather than a multi-component mixture.

ACKNOWLEDGEMENTS

H. Scott Fogler initiated the departmental effort to incorporate open-ended problems in the curriculum, and Brice Carnahan originally identified the *New York Times* article referenced in this paper as the basis for a problem in reaction engineering. Tom Thornton performed the literature search and obtained the kinetics data used in this open-ended problem.

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ChE book review

POLYMER CHEMISTRY: AN INTRODUCTION

(Second Edition)

Raymond B. Seymour and Charles E. Carraher, Jr.
Marcel Dekker, Inc., New York, 10016
720 pages, \$45.00 (1988)

Reviewed by
William J. Koros
The University of Texas

This book is an updated version of a text which was first published some years ago by McGraw-Hill. This second edition comprises the eleventh volume in a series of undergraduate texts dealing with a broad range of topics in chemistry. As is pointed out in the forward to the book, written by Herman Mark, this new edition is quite up-to-date in terms of topical coverage, but without unnecessary complications. The book is easily read and has an almost conversational tone to it. One can imagine sitting across from the two authors (whose broad knowledge of polymer science is well-known) and having the book unfold in a casual, but still logical, fashion.

The revised text includes a number of new topics, and the authors note that the book meets the ACS guidelines for topical coverage in an introductory polymer chemistry course. A glossary and series of questions related to the material is given at the end of each chapter. The questions at the end of the chapter are a plus for the book since it is difficult to obtain good homework exercises in the polymer field without actually synthesizing them oneself. Nevertheless, while these exercises are useful, they are mostly discussable in nature and do not satisfy the persistent need for a really good compilation of computational problems to illustrate principles discussed in a polymer text.

As must be the case whenever one considers a wide range of topics and is committed to keeping the page-count within bounds, none of the topics is treated in any detail. The title, *Polymer Chemistry*, is not

Continued on page 167.