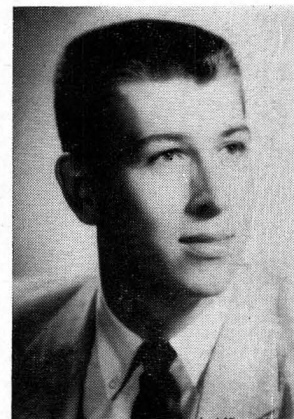


## TOWARD A CONTEMPORARY COURSE IN GRADUATE KINETICS AND REACTOR DESIGN

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There are a number of intermediate size Universities today which are offering graduate programs in Chemical Engineering. One common characteristic of many of these schools is their limited supply of technical experts throughout the University in all areas of contemporary technology. At the same time, the Chemical Engineering faculty has a responsibility to the graduate student to present up-to-date graduate courses which consider contemporary topics and material. It is also common to find a limited graduate enrollment such that well-defined special topics courses cannot be offered to cover such subjects specifically.

To meet this need, the University of Toledo offered a one-semester graduate course in kinetics and reactor design which selected a few of these contemporary subjects and integrated them into a Master's level course. The topics chosen were non-ideal mixing and residence time distribution, biochemical kinetics, polymerization kinetics and reactor design, and heterogeneous kinetics and reactor design. (It should be mentioned that at the Doctorate level a separate course is offered in heterogeneous kinetics and reactor design). Obviously, the purpose of the course was not to develop expertise in the field, but rather to extend the student's undergraduate kinetics into more advanced and topical areas. The particular subjects chosen were based primarily on departmental and student research interests. Other topics such as electrochemical kinetics, fuel cells, photochemical reactor design, plasma arc high temperature kinetics, etc., are examples of other equally appropriate areas. The primary objective of the course was to expose the student to a number of advanced areas in which kinetic analysis and reactor design have application and that the basic concepts are inter-related. This approach of topic integration has been exemplified in the areas of heat, mass and



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TABLE I—COURSE OUTLINE FOR AN INTEGRATED KINETICS AND REACTOR DESIGN CLASS

1. **Review of Basic Concepts**
  - a) Equivalent of first eight chapters of "Chemical Reaction Engineering," Levenspiel, Wiley, New York (1962).
  - b) Vector analysis approach to transport equations as per "Transport Phenomena," Bird, Stewart and Lightfoot, Wiley, New York (1963).
2. **Non-ideal mixing**
  - a) Residence time distribution measurements.
  - b) Alternative math models to describe real systems.
  - c) Experimental study with 25 gallon CSTR.
3. **Heterogeneous kinetics and reactor design (gas-solid systems.)**
  - a) Physical and chemical adsorption.
  - b) Microporous catalysts (surface area measurement and pore diffusion).
  - c) Active site gas-solid kinetic models.
  - d) Fixed bed reactor design (isothermal case only).
4. **Polymerization kinetics and reactor design**
  - a) Kinetics of free radical and condensation polymerizations.
  - b) Heat transfer problems.
  - c) Case study (suspension PVC process).
5. **Biochemical Kinetics (enzyme systems).**
  - a) Kinetic models for enzyme kinetics.
  - b) Michaelis-Menten equation.
  - c) pH effects.

momentum transfer by the now classic "Transport Phenomena" by Bird, Stewart and Lightfoot. Chemical reaction engineering does not at present enjoy such a beautiful single treatment of the subject as an integrated phenomena.

Other approaches to graduate courses in this area are perhaps more conventional in that they usually concentrate on a particular aspect of kinetics or reactor design. For example, J. J. Carberry recently published (This journal, Sp '68) an outline for a graduate course in Chemical Reaction Engineering. The course, as he pointed out, is about 75% devoted to heterogeneous reaction-reactor problems. There are many other areas of equal importance which a Master's candidate student should appreciate, particularly if he is taking only one course in graduate kinetics and reactor design. More detailed emphasis of specific topics might better be spared for Doctorate level or special topics courses. Consideration should be given to the fact that many of the Master's degree students will not be working directly with heterogeneous kinetics problems. There is a greater probability, however, that a working knowledge of kinetics and reactor design in such areas as water pollution, plastics, and heterogeneous systems in general will involve a greater majority of the students upon graduation.

#### COURSE OUTLINE

The outline of the course shown in Table 1 represents an attempt to integrate kinetically related topics within one graduate course. The choice of subjects was admittedly somewhat arbitrary, but could easily be altered if so desired.

Approximately one month was allotted per topic, which for a three credit-hour course gave about twelve student-contact hours per area. The students were given current journal articles for analysis and critique as take-home exams in each of the topics, except non-ideal mixing where they mathematically analyzed laboratory residence time-distribution data which they took on a 25 gallon CSTR. This procedure spared class time for lecture and discussion and also forced the students to apply their knowledge.

Material for the course came from a variety of texts and literature articles. A few of the references are listed in Table II.

The references given here were those primarily used to develop the course. Others of lesser importance were used when appropriate, but those

listed are quite satisfactory for the complete development of the course. The material in these references is sufficiently concise and well-written that an instructor interested in kinetics and reactor design should not encounter any difficulty in developing the course. It does not require expertise in all areas.

At a first glance, this may seem like an over-ambitious approach, both for the students and the professor. Previous experience, however, showed that the material could be covered in some depth and that the students were not overburdened. There are a number of areas with common elements which make the concepts easier to present. For example, the steady-state assumption made in free-radical kinetics is also used in enzyme kinetics. Once the student grasps the basic concept, transfer to other areas is both easy and logical.

TABLE II. — SUGGESTED REFERENCES FOR COURSE

#### Non-ideal mixing

Bischoff and McCracken, "Tracer Tests in Flow Systems," *I&EC* 58, No. 1, p. 18 (1966).

Levenspiel, "Chemical Reaction Engineering," Chapter 9, Wiley & Sons, N. Y., (1963).

Wolf and Resnick, "Residence Time Distribution in Real Systems," *I&EC Fund.*, 2, No. 4, p. 287 (1963).

#### Heterogeneous kinetics and reactor design

Corrigan and Mills, "Catalytic Reactor Design," CE Refresher Series, Part IX, McGraw-Hill, (1956).

Froment, "Fixed Bed Catalytic Reactors," *I&EC*, 59, No. 2, p. 18 (1967).

Hougen and Watson, "Chemical Process Principles," Part III, Kinetics and Catalysis, Wiley & Sons, N. Y., (1964).

Petersen, "Chemical Reaction Analysis," Prentice-Hall, N. J., (1965).

#### Polymerization kinetics and reactor design

Albright, "Vinyl Chloride Polymerization by Suspension Processes Yields Polyvinyl Chloride Resins," *Chem. Eng.*, June 5, p. 145 (1967).

Billmeyer, "Textbooks of Polymer Chemistry," Interscience Publishers, N. Y., (1966).

Flory, "Principles of Polymer Chemistry," Cornell U. Press, Ithaca, N. Y., (1953).

Tanford, "Physical Chemistry of Macromolecules," Wiley & Sons, N. Y., (1960).

#### Biochemical Kinetics

Amdur and Mammers, "Chemical Kinetics: Principles and Selected Topics," Chapter 7, Enzyme Kinetics, McGraw-Hill, N. Y., (1966).

Arba, Humphrey and Millis, "Biochemical Engineering," Academic Press, N. Y., (1965).

King and Altman, "A Schematic Method of Deriving the Rate Laws for Enzymecatalyzed Reactions," *J. Phys. Chem.*, 60, p. 1375 (1965).

## CONCLUSION

The purpose of this article has been to present a case for upgrading the graduate chemical engineering course in kinetics and reactor design, particularly for the intermediate size schools which cannot support the development of more sophisticated courses in all of the contemporary areas. The course outline presented is an example of a successful program presented as a one-semester course at the University of Toledo. Selections of the course can obviously be changed to accommodate the needs and interests of students and faculty.

If sufficient interest is shown to support the expansion of one of the areas in particular, it could be given as a special topic course or as a seminar. Graduate students in the Chemistry Department should also be contacted as potential candidates for such courses.

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campus. Generally this requires that they be trained side by side with majors in chemistry rather than be placed in service courses with non-chemists. It is important not only that the chemistry training be up-to-date but also that it be used in the subsequent chemical engineering courses. This means that the chemical engineering staff too must keep itself informed on modern chemistry." Those ideas are excellent, but in keeping up with chemistry, we must insist that chemistry keep up with itself. Also we as chemical engineers must see that the chemistry training is used in the subsequent chemical engineering courses. We have no other choice.

## SUMMARY AND CONCLUSIONS

The conclusion is that we must change our style in chemical-engineering education. If we do not, we will not as chemical engineers make the contribution to society that we must. A good fraction of our goal is to provide people who have the ability to work in the area of optimum control of chemical reactions for the benefit of mankind. If we are not careful, we will lose that ability and even franchise to deal with one of the most important needs of society. How do we meet our responsibility? Specifically, the following changes are suggested as the avenue to capture our new style:

1. A two-year course in chemistry be given by the chemistry department, for chemists and engineers alike, in which inorganic and organic chemistry are combined in the framework of physical chemistry. Appropriate laboratory work would be given, with required experiments plus optional experiments which would be of special interest to the student as he looks ahead to his future.

2. There be a requirement that all engineering and science students take the two-year course in chemistry.

3. A real association of the first two years of physics and chemistry be effected.

4. A third-year course in applications of physical chemistry be taught by the chemical-engineering faculty. This third-year course would focus upon the first two years of chemistry and consider chemical principles in terms of applications in real systems. In this course, modern chemistry and classical physical chemistry would be combined in the study of applications. A course of this type probably will not be taught in the framework of chemistry's interest in these days. The responsibility is ours, and we must meet it.

5. Major emphasis on chemical change be established in the transport change.

6. A senior course in design be more encompassing than envisioned to date. It should be a course with a title such as "Design, Simulation, and Control of Chemical Processes." This course would bring together the students' training in chemistry with added information in industrial chemistry, process dynamics, applied mathematics applied mechanics, and other areas of engineering endeavor. In particular the focus would still be control of chemical change.

7. Cooperative teaching of key courses be introduced as a must in engineering training and especially in chemical engineering. There is no reason today for a compartmentalization of courses and especially no reason for use of the older style of tandem teaching of courses of mutual interest. Rather courses of mutual interest must be taught in a mutual way. In the interest of conserving time and improving quality of education, the cooperative teaching must expand in a way that we really do not even dream of at this moment. The cooperative teaching requires not only cooperative effort within a school but cooperation between schools such as engineering and medicine.

8. There be a fourth-year, all-engineering laboratory with elective experiment in chemical change.

Finally, it is necessary to emphasize that our curriculum efforts are obsolescent, not obsolete, and that our profession is not obsolescent but very much alive. We must make changes, nevertheless, in our programs that we have not dared to make before. We must elicit the cooperation of all parts of our schools. These changes are not changes that can be made internally in the departments of chemical engineering; they encompass the attitude of the whole university. Let us not be shaken by such a goal and step ahead and lead, because we have a unique position of leadership in our concern with chemical change.