A Course in

COAL LIQUEFACTION PROCESSES

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It is the purpose of this course to provide a comprehensive background to coal liquefaction in order to prepare the student intent upon a career in a coal-related field.

OF ALL THE EFFECTS generated by the oil crises of recent years, the most positive has been the invigoration of research and development of alternative energy sources. The U. S. Department of Energy has been a prime mover in stimulating university activity in this area by funding research. However, the academic institutions themselves have, as yet, failed to reflect the concern over and urgency of this activity in their curricula. It was this need for updating university offerings that prompted T. D. Wheelock to publish his outline of "A Course in Coal Science and Technology" in a recent issue of *Chemical Engineering Education*. In a similar vein, the ChE Department of the University of Southern California has produced a new course in Coal Liquefaction Processes. It is hoped that this outline will serve as a reference to other educators in establishing similar courses.

Teh Fu Yen obtained his B.S. from Central China University, M.S. from West Virginia University and Ph.D. from Virginia Polytechnic Institute. His principle research intent in recent years is in fossil fuels, their extractions, conversions, as well as their environmental control technology. He has lectured extensively at major oil companies worldwide and has authored over 160 technical papers and edited nine books. He is the editor of **Energy Sources** as well as the editor of **Biomaterials, Medical Devices and Artificial Organs.** He has been associate professor of Chemical Engineering at the University of Southern California since 1971.

From its first offering in the Fall of 1977, the graduate course drew keen interest, with 20 students enrolling and a number of others auditing. On the average, 75% of the enrollees have been graduates in the ChE program, although graduate students from Mechanical, Petroleum, and other engineering and chemistry disciplines have been attracted to the course. The enrollment prerequisite is a B.S. in Physical Science or Engineering. Some of the students participated in the class via USC's Interactive Instructional Television program, which allows students in neighboring industries to have a two-way communication with a live broadcast of the class.

A great deal of research is currently focused on the production of synthetic fuel from coal. The abundant reserves of coal in the United States makes the enterprise attractive, and concrete strides in Poland and Germany have created confidence in the eventual realization of the process. The state-of-the-art technology is the present problem, though.

It is the purpose of this course to provide a comprehensive background to coal liquefaction in order to prepare the student intent upon a career in a coal-related field. The author feels that the way to serve the pursuit and the best interests of the nation, is to insure that trained technical manpower is available for research. Class coverage includes coal chemistry and physics, coal petrography, coal types, carbonization, hydrogenation, Fischer-Tropsch synthesis, solvent refining, and other processes and aspects. The one-term course is composed of 16 two-and-a-half hour lectures (Table 1).

Since the technology is not established, there is no textbook for the teaching of the course.

This fact has been a major cause in keeping such a course out of university curricula. However, to remedy this situation, a massive literature search was conducted during the spring and summer prior to the first offering of the course. Besides gathering material known to the author, over 240 specialists in industry, educational institutions, and government agencies in this country and abroad were solicited for useful papers, charts, illustrations, and other literature relevant to the subject. The response was voluminous. The resulting body of papers, publications, and suggestions received from our correspondents created a pool of information which gives full representation of the current state of coal liquefaction. The vast amount of material was collated, overlapping material was eliminated, it's relative importance was weighed, and, finally, sixty-four papers (roughly separable into sixteen different topic headings) were selected (Table 2). This textual material was supplemented by a book list which effectively covers the groundwork essential to understanding the subject.

TABLE 1
Lecture Topics

1. Introduction—Coal Resources and Supplies; Coal Mining Technology Development
2. Origin of Coal; Coal Types and Ranks; Petrography; Metamorphism
3. Coal Chemistry; Coal Reaction; Coal Structures
4. Physical Properties of Coal: Statistical Approaches and Structural Parameters
5. Coal Preparation; Comminution; Coal Feed Engineering Problems
6. Thermal Pyrolysis of Coal; Kinetics and Mechanism of Thermal Decomposition
7. Carbonization; Mesophase; Cokes
8. Solubility Parameters; Solvent Refining; Nature of Hydrogen Donors
9. Catalysis; Catalytic Hydrogenation
10. Fischer-Tropsch Synthesis—Generalized Gasification
11. Coal Liquids; Separation and Isolation of Asphaltenes; Characterizations
12. Refining, Upgrading, Desulfurization, Demetallization, Denitrogenation
13. Coal-Derived Chemicals and Products; Other Synfuels
14. Novel Approaches; In-Situ Production
15. Environmental, Safety, and Health Problems in Coal Conversion
16. Process and Reactor Design; Mathematical Models; Reaction Control

LECTURES

THE WEEKLY LECTURES have been primarily delivered by the instructor. Because of the interdisciplinary nature of the course, careful control has been exerted in order to keep the overall objective in clear view, and to keep the course from being diverted into the other disciplines which are touched upon tangentially (such as mining and mechanical engineering, chemistry, and geology). Occassionally, a guest lecturer is invited, but this is not a general feature of the course's format.

The first five lectures lay the groundwork necessary to an understanding of coal. They explore a number of topics, including the derivation of coal and much coal science. Lectures 6 through 10 explore the major liquefaction processes in detail. Included are thermal pyrolysis, carbonization, catalytic hydrogenation, and Fischer-Tropsch synthesis, as well as others. The following group of lectures concerns the product of liquefaction: coal liquid. The final three lectures look toward the future, discussing liquefaction processes still in development and projecting future technology, along with environmental and health impacts.

For class preparation the students read four related papers which are held on reserve in the library.

CLASS WORK

CLASS WORK IS COMPRISED of three categories which carry equal weight in the calculation of grades: homework problems, term paper, and tests.

Three times throughout the semester, sets of homework problems are distributed to the students. Usually, the sets contain five problems whose solutions require quantitative and analytic calculations. An example is: Calculate the thermal efficiency (or the overall efficiency) for Fischer-Tropsch Synthesis. The student would arrive at a value by applying design criteria to chemical principles and data conveyed in class. The home-

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work serves a dual purpose: to illustrate chemical engineering principles and to put into practice formulas and data given in class.

In assigning topics for term papers, the student "nominates" three possible subjects in the order of his preference. The instructor makes the final selection; in this way, control is exerted to insure that papers do not duplicate topics. This is desirable, because later in the semester students present detailed outlines of their papers before the class. In this way, students (as auditors) are exposed to new material and are asked to question the soundness of the various theses, and (as presenters) are made to cogently deliver and defend their works.

The term papers are not exhaustive literature surveys, but rather, are the students assessments of various aspects of coal liquefaction. Creativity is stressed, and the student is encouraged to organize and substantiate his or her own ideas on the subject, as well as to draw from interest or background in other related disciplines in the formulation of an original and personal position. Two such student papers, resulting from the first offering of the course, were subsequently published in technical journals, attesting to the relevance of such work.

The midterm and final examinations are composed of problems requiring quantitative and analytic solutions, much like the homework problem cited above.

As an adjunct to classwork, an open invitation to participate in university research projects is extended to the students. This is made possible by a number of continuing coal research contracts from DOE for which the author is the principal investigator.

STUDENT POLL

DUE TO THE STILL-EVOLVING nature of coal liquefaction technology, university courses on the subject must wage a battle on two fronts: striving to keep abreast of the changing face of the field, and seeking out the class format and material which will best serve the subject. End-of-semester student polling is a standard procedure at the University of Southern California and the author has had a more than customary interest in student reactions and suggestions, with a view to shaping the best possible course offering.

. . . the student responses were heartening. The majority of the class members remarked very favorably on the worth and success of the course.

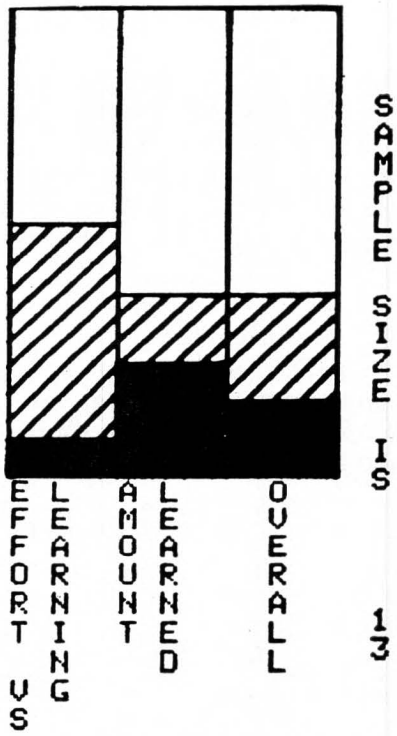

FIGURE 1. Graphic Representation of Student Response to Course

Taking one representative semester, the 18 enrolled classmembers were asked to complete a course evaluation form anonymously, and 13 (or 72%) complied. The questionnaire and method of interpretation applied to it were developed by Dean Frederic Carlson, Jr., Director of USC's Engineering Computer Laboratory. The graphic representation of the student response to the course is presented in Figure 1. In brief, the questionnaire responses are interpreted for three categories: effort vs. learning, amount learned in the course, and overall rating. Each category of responses is represented by a bar graph in which black areas represent responses which are characterized as "poor," crosshatched areas signify "average," and white "excellent."

In the evaluation category of effort vs. learning for our course, six students responded that the material was enjoyable and stimulating. Six were satisfied with what they learned in view of the effort exerted and only one found himself struggling to get through the course rather than attempting to learn.

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In the category of amount learned in the course, 8 students felt that they had learned a great deal, 2 had learned an adequate amount, and 3 felt they had learned very little. The overall rating was very similar, with 8 giving a rating of excellence, three average, and two poor.

Moreover, the student responses were heartening. The majority of the class members remarked very favorably on the worth and success of the course. The lack of a textbook drew several responses, most feeling that when a textbook does become available the course will be better served. The large body of reading prompted comments ranging from "challenging" to "hard and laborious." It is unfortunate that no such text exists, and this is something which should be rectified as soon as possible. Until then, a collection of papers seems to be the only adequate substitute, as undistilled and inconcise as it is. □

TABLE II
Course Reading List
(Arranged Under Lecture Headings)

INTRODUCTION—COAL RESOURCES AND SUPPLIES, COAL MINING TECHNOLOGY DEVELOPMENT

1. J. A. Barlow, "Coal Mining" in Coal and Coal Mining in West Virginia, Coal Geology Bull. No. 2, 1974.
2. M. King Hubbert, "Survey of World Energy Resources" in Energy and the Environment, Cost-Benefit Analysis, (R. A. Karam and K. Z. Morgan, ed.) Pergamon, 1976 pp. 3-36.
3. B. L. Sagmiller and J. E. Wilson, "Mining of Fossil Hydrocarbons", Chem. Eng. Prog. (Symposium series No. 85) 64, 51-56 (1968).
4. G. T. Fettwers, "Contribution to the Assessment of World Coal Resources or Coal is Not So Abundant," in Energy Resources (M. Gonon, ed.) pp. 467-530 (1976).

ORIGIN OF COAL; COAL TYPES AND RANKS; PETROGRAPHY; METAMORPHISM

1. A. Davis, W. Spackman and P. H. Given, "The Influence of the Properties of Coals on Their Conversion into Clean Fuels", Energy Sources 3(1) 55-81 (1976).
2. B. C. Parks, "Origin, Petrography and Classification of Coal", in Chemistry of Coal Utilization, Supplementary Volume (H. H. Lowry, ed.) pp. 1-34, 1965.
3. W. Francis, "The Origin of Coal", in Coal—It's Formation and Composition, Chapter 1, 1961.
4. W. Spackman, "The Maceral Concept and the Study of Modern Environments as a Means of Understanding the Nature of Coal", Trans. New York Acad. Sci., 20 411-423 (1958).

COAL CHEMISTRY, COAL REACTION, COAL STRUCTURES

1. S. K. Chakrabarty, "Organic Chemistry of Coal and Chemical Oxidation", The Fundamental Organic Chemistry of Coal, Proceedings, pp. 89-104 (1975).
2. F. R. Majo, J. Huntington, and N. Kirshen, "Oxidation of Coal, Coal Fractions, and Coal Models", Preprint, 1976 Coal Chemistry Workshop, pp. 189-201 (1976).
3. H. J. Gluskoter, "Mineral Matter and Trace Elements in Coal", Trace Elements in Fuel (S. P. Babu, ed.), pp. 1-22 (1975).
4. T. F. Yen, "Chemical Aspects of Interfuel Conversion", Energy Sources, 1, 117-136 (1973).

PHYSICAL PROPERTIES OF COAL, STATISTICAL APPROACHES AND STRUCTURAL PARAMETERS

1. H. Tschamler and E. de Ruiter, "Physical Properties of Coals", Chapt. 2 in Lowry's Chemistry of Coal, Utilization (supplementary), Wiley, 1963, p. 35.
2. H. L. Retcofsky, "Spetrometric Investigations of Coal", in The Fundamental Organic Chemistry of Coal, 1975, pp. 59-79.
3. M. Oka, H. C. Chang and G. R. Gavalas, "Computer-assisted Molecular Structure Construction for Coal-derived Compounds", Fuel, 56, 3 (1977).
4. T. F. Yen, "Resonance Topology of Polynuclear Aromatic Hydrocarbons", Thoret. Chim. Acta, 20, 399 (1971).

COAL PREPARATION, COMMINUTION, COAL FEED ENGINEERING PROBLEMS

1. R. C. Neavel, "Coal Plasticity Mechanism: Inferences from Liquefaction Studies," Proc. Coal Agglomeration and Conversion Symposium, WRU, pp. 119-133, 1976.
2. Duane Skidmore, "Agglomeration as a Factor in the Non-Catalytic Liquefaction of Coal," Proc. Coal Agglomeration and Conversion Symposium, WRU, pp. 135-145, 1976.
3. W. Francis, "Coal Preparations-Grading and Crushing" and "Coal Cleaning Representations of Washer Performance", Fuels and Fuel Technology, Vol. 1, pp. 55-87, 1965.
4. P. Howard, A. Hanchett and R. G. Aldrich, "Chemical Communication for Cleaning Bituminous Coal", Cleaning Fuels from Coal Symposium II Papers, Institute of Gas Technology, pp. 733-750, June 1975.

THERMAL PYROLYSIS OF COAL, KINETICS AND MECHANISM OF THERMAL DECOMPOSITION

1. H. C. Howard, "Pyrolytic Reactions of Coal," in Lowry's Chemistry of Coal Utilization (Supplementary Volume) Wilby 1965, pp. 340-384.
2. H. W. Sternberg, R. Raymond and F. K. Schweighardt, "The Nature of Coal Liquefaction Products," Preprint, ACS Chicago Meeting, Aug. 1975, pp. 198-209.
3. R. T. Eddinger, "Pyrolysis to Coal Conversion", Paper at World Coal Conference, London, England, Sept. 1975.
4. C. S. Wen and T. F. Yen, "Optimization of Oil Shale Pyrolysis", Chem. Eng. Sci., 32, 346-349 (1977).

CARBONIZATION, MESOPHASE, COKES

1. N. Y. Kirov, J. M. O'Shea and G. D. Sergeant, "The Determination of Solubility Parameters for Coal", Fuel (London), 46, 415-424 (1967).
2. D. W. van Krevelan, "Chemical Structure and Properties of Coal, XXVIII—Coal Constitution and Solvent Extraction", Fuel (London), 44, 229-242 (1965).
3. Battelle Energy Program Report "Solvent Refining Processes in Liquefaction and Chemical Refining of Coal, 1974, pp. 14-28.
4. J. M. Angelovich and H. F. Silver, "A Study of Solvents" for the Liquid Phase Conversion of Coal", Reprint 10B, AIChE, 61 Annual Meeting, 1968.

SOLUBILITY PARAMETERS, SOLVENT REFINING, NATURE OF HYDROGEN DONORS

1. J. L. White, "Mesophase Mechanisms in the Formation of the Microstructure of Petroleum Coke," ACS Symposium Series, No. 21 (1975).
2. J. E. Zimmer and J. L. White, "Disclinations in the Carbonaceous Mesophase," Mol. Cryst. Liq. Cryst., 38, 177-193 (1977).
3. R. W. Shoenberger, "Formcoke Preparation in Clean-Coke Process", ACS Preprint, Div. Fuel Chem. 20(4), 46-69 (1975).
4. A. Sass, "The Production of Liquid Fuels from Coal", Minerals Sci. Eng. 4(4),pp. 18-27, (1972).

CATALYSIS, CATALYTIC HYDROGENATION

1. VanKrevlen "Chemistry of Coal Hydrogenation", in Coal, Elsevier, 1961 p. 201-218.
2. J. L. Cox "Catalysts for Coal Conversion", Clean Fuels from Coal, 1973 Symposium, IGT, pp. 271-297.
3. G. C. A. Shuit and B. C. Gates, "Chemistry and Engineering Catalytic Hydrodesulfurization", AIChE Journal, 19(3), 417 (1973).
4. W. H. Wiser, "Some Chemical Aspects of Coal Liquefaction", Coal Workshop, Penn State, 1975.

FISHER-TROPSCH SYNTHESIS—GENERALIZED GASIFICATION

1. H. Pichler and A. Hector, "Carbon Monoxide-Hydrogen Reactions" in Encyclopedia of Chemical Technology, Kirk-Othmer, 2nd ed., Vol. 4, 446-489 (1964).
2. G. A. Mills and F. W. Steffgen, "Catalytic Methanation", Catalysis Rev. 8, 159 (1973).
3. J. B. O'Hara, N. E. Jantz and R. V. Teeple "Conversion of Coal to Liquids by Fischer-Tropsch and Oil/Gas Technologies", ACS Div. Fuel Chem., Preprint, 22(7), 20 (1977).
4. K. H. Hedden, "Coal Gasification," in Alternative Energy Sources (J. P. Hartnett, Ed.), Academic Press, 1976. pp. 111-148.

COAL LIQUIDS, SEPARATION AND ISOLATION OF ASPHALTENES, CHARACTERIZATIONS

1. H. N. Sternberg, R. Raymond and F. K. Schweighardt, "Acid-Base Structure of Coal-Derived Asphaltenes", Science, 188, 49 (1975).
2. I. Schwager and T. F. Yen, "Separation of Coal Liquids from Major Liquefaction Processes in Meaningful Fraction," in Liquid Fuel from Coal, (R. T. Ellington, ed.), Academic Press, 1977, pp. 233-248.
3. M. Farcasiu, T. O. Mitchell, and D. D. Whitehurst, "On the Chemical Nature of the Benzene Insoluble Components of Solvent Refined Coals," A.C.S. Div. Fuel Chem., Preprint, 217, 11 (1976).
4. T. F. Yen, "Chemistry of Asphaltene in Coal Liquids," in Preprint, Workshop on Coal Chemistry, Stanford Research Institute, 1976, pp. 144-164.

REFINING, UPGRADING, DESULFURIZATION, DEMETALLIZATION, DENITROGENERATION

1. R. A. Meyers, "Chemistry of Desulfurization Reactions" in Coal Desulfurization, Marcel Dekker, Inc., Chapter 3, 1977.
2. W. K. T. Gleim, "Role of Asphaltenes in Refining", in Bitumens, Asphalts and Tar Sands, Development in Petroleum Science, Vol. 7 (G. V. Chilingar and T. F. Yen, ed.) Elsevier, Chapter 10, 1978.
3. E. Gorin and H. E. Lebowitz, "Recovery Sulfur and Mineral Matters from Coal," Chem. Eng. Prog. 64-68 (1974).
4. G. A. Mills and H. Perry, "Fossil Fuel → Power + Pollution", Chem. Tech., Jan. 1973, pp. 53-63.

COAL-DERIVED CHEMICALS AND PRODUCTS, OTHER SYNFUELS

1. A. M. Squires, "Chemicals from Coal", Sci. 191, 689-700 (1976).
2. G. A. Mills and B. M. Harney, "Methanol—The "New Fuel" from Coal", Chem. Tech., 4(1), 26-31 (1974).
3. J. B. O'Hara, E. D. Becker, N. E. Jentz and T. Harding, "Potential for Petrochemical Feedstocks and Chemicals from Coal," AIChE Meeting 82nd National Meeting, 1976. Symposium on Chemicals from Coal—New Frontiers.
4. H. G. Davis, "Coal as a Raw Material for the Chemical Industry," Fourth Annual Illinois Energy Conference, Chicago, IL, 1976.

NOVEL APPROACHES, IN SITU PRODUCTION

1. D. V. Keller, Jr. and C. D. Smith, "Spontaneous Fracture of Coal", Fuel (1977).
2. W. K. Sawyer, "Reviewing Current UCG Model Capabilities", Proceedings of 2nd Annual UCG Symposium, MERC, 1976, pp. 477-488.
3. D. R. Skidmore and C. J. Konya, "Liquefaction Study of Several Coals and a Concept for Underground Liquefaction", Proc. Coal Agglomeration and Conversion Symposium, WVU, 1976.
4. G. A. Mills, "Catalytic Chemistry of New Syn Fuels Processes", I.E.A. Coal Science Conference, Coal Research Establishment, England, 1977.

ENVIRONMENTAL PROBLEMS IN COAL CONVERSION, ASPECTS OF SAFETY AND HEALTH

1. Harry Perry, "Environmental Aspects of Coal Mining", in Power Genrations and Environmental Change (D. A. Berkeowitz and A. M. Squires, ed.) MIT Press, 1971, pp. 317-339.

2. G. N. Reddy, "Environmental Aspects of Coal Conversion Plant Siting and Cost of Pollution Control", Third Annual International Conference on Coal Gasification and Liquefaction, Pittsburgh, Pa., August, 1976.
3. R. G. Lett, C. E. Schmidt, R. R. De Santis and A. G. Sharkey, Jr., "Screening for Hazardous Elements and Compounds in Process Streams of the 1/2 Ton Per Day Synthoil Process Development Unit", PERC RI 77/12, 1977.
4. B. I. Loran and J. B. O'Hara, "Specific Environmental Aspects of Fischer-Tropsch Coal Conversion Technology", Third Symposium on Environmental Aspects of Fuel Conversion Technology, Hollywood, Florida, Sept. 1977.

PROCESS AND REACTOR DESIGN, MODELS, REACTION CONTROL

1. C. Y. Wen, "Optimization Studies of Various Coal-Conversion Systems", ERDA Reports FE-2274-2, 1976.
2. Y. P. Hsia and T. F. Yen, "Evaluation of Coal Liquefaction Efficiency Based on Various Ranks", Energy Sources, 3(1)39 (1976).
3. C. Y. Wen and K. W. Han, "Kinetics of Coal Liquefaction", ACS, Div. Fuel Chem., 20(11), 216 (1975).
4. P. Wellman and S. Katell, "The Economics of Coal Conversion Systems", SPE Paper 5097 (1974).

TABLE III
Supplementary Course Reading List

ACS, "Coal Science," Advances in Chemistry Series 55, Washington, D C., 1966.
AIChE, "Coal Processing Technology," Chemical Engineering Progress,
AIChE, "Coal Processing Technology, Volume 2," Chemical Engineering Progress,
Ellington, R. T., (ed.), "Liquid Fuels from Coal," Academic Press, San Francisco, 1977.
Elliott, M. A., (ed.), "Chemistry of Coal Utilization, Second Supplementary Volume," Wiley, New York, 1963.
Francis, W., "Coal, Its Formation and Composition," Edward Arnold, London, 1961.
Howard-Smith, I. and G. J. Werner, "Coal Conversion Technology," Noyes Data Corp., Park Ridge, New Jersey, 1976.
IGT, "Clean Energy Fuels from Coal, Symposium II Papers," 1975.
Katzer, J. K. and B. C. Gates, "Catalytic Processing in Fossil Fuel Conversion," AIChE Today Series,
Lowery, H. H., (ed.), "Chemistry of Coal Utilization, Vol. I and II, Wiley, New York, 1945.
Lowery, H. H., (ed.), "Chemistry of Coal Utilization, Supplementary Volume," Wiley, New York, 1963.
Tetra Tech, Inc., "Energy from Coal, a State-of-the-Art Review," U.S. Printing Office, Washington, D.C., 1976.
Van Krevelen, D. W., "Coal, Typology—Chemistry—Physics—Constitution," Elsevier, New York, 1961.
William, D. A. and G. Jones, "Liquid Fuels," Pergamon, Elmsford, N. Y., 1963.

IN MEMORIUM

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had a strong influence on chemical engineering in the United States where a majority of departments of chemical engineering use it as a text. It has also been published in Hungarian, 1961, as an International Students Edition in Tokyo in 1962 and 1968, and in Spanish in 1973. He also contributed to Perry's Chemical Engineering Handbook and the Encyclopedia of Engineering and Sciences.

During his career he published more than seventy technical papers primarily dealing with mass transfer and mass transfer operations. His research interests included liquid-liquid extraction, distillation, absorption and mixing in multiphase systems. His most recent research centered on mass transfer in baffled and unbaffled agitated vessels and three phase mixing in agitated full baffled columns and vessels. He was honored for his teaching with the George Westinghouse award for Distinguished Engineering Teaching by the ASEE in 1957. In 1963 he was the recipient of the William H. Walker Award for outstanding contributions to the chemical engineering literature, awarded by AIChE. In 1968 and again in 1970 he received additional teaching awards, first from the NYU Alumni and then from the Manufacturing Chemists Association.

Dr. Treybal was a fellow of the American Institute of Chemical Engineers, the New York Academy of Science and the American Institute of Chemists. He was a long time member of the American Chemical Society and the American Society for Engineering Education. He was a member of Sigma Xi and Tau Beta Pi Honor Societies. He was also a registered professional engineer in both New York and Rhode Island.

His former dean at NYU, John Ragazzini, remembered him as "a superb technical person with enviable human qualities." Part of his human qualities showed through his interest in art and music. He had an intense interest in opera and was a fine artist.

The students and faculty have started a memorial fund in his name at the University of Rhode Island. They hope to honor his name and tradition with an endowed chair at the University of Rhode Island.