Final Project Report

Project Title:	New Process Modelling, Design, and Control Strategies for Energy Efficiency, High Product Quality, and Improved Productivity in the Process Industries
DOE Award Number:	DE-FG02-86ER13551
Project Investigator:	W. Harmon Ray
Organization:	University of Wisconsin
Project Consortium/ teaming members:	NONE

Executive Summary

The process industries in the U. S. are facing stiff competition in the world market because of locally high labor rates, tight environmental standards, and older technology for many processes. This project was concerned with the development of process design and control strategies for improving energy efficiency, product quality, and productivity in the process industry. In particular, (i) the resilient design and control of chemical reactors, and (ii) the operation of complex processing systems, was investigated. Major emphasis in part (i) was on important classes of chemical reactors: packed bed reactors and polymerization processes. In part (ii), the main focus was on developing process identification and control procedures which allow the design of advanced control systems based on limited process information and which will work reliably when process parameters change in an unknown manner. Specific topics studied included new process modeling procedures, nonlinear controller designs, and control strategies for multiunit integrated processes. Both fundamental and immediately applicable results were obtained. The theoretical developments were tested experimentally on pilot scale equipment in our laboratory. The new design and operation results from this project were incorporated into computer-aided design software and disseminated to industry. The principles and design procedures have found their way into industrial practice.

Project Personnel

The principal investigator was the only faculty or research staff member involved. The other research personnel were graduate students and postdoctoral researchers.

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<u>Project Overview</u>

Specific Project Objectives:

It was expected that there would be valuable fundamental as well as immediate applicable practical results arising from this study. We classified the specific objectives under each of the various parts of the research project.

(1) Resilient Design and Control of Chemical Reactors

These investigations were expected to provide:

(a) New quantitative criteria and design procedures for static and dynamic resilience of highly nonlinear chemical reactors.

(b) Special insight into the application of these criteria to crucial chemical reactors of the following types:

(1) Several types of batch and continuous polymerization processes.

(2) Packed bed reactors.

(c) The development of new sensors for monitoring polymer properties and quantitative predictions of the effect of new sensors on quality of control for all of the reactors studied.

(2) Operation of Complex Processing Systems

This part of the project was dedicated to establishing new, workable, and robust control strategies to deal with the problems arising most frequently in process control. The research was expected to provide:

(a) The development of new process modeling, state estimation, and robust controller design procedures which rely only on data normally available from the process. These procedures should allow a standard approach to process monitoring and control of multivariable systems.

(b) New techniques for the control of nonlinear processes such as chemical reactors.

(c) New, easily applied, general purpose procedures for the design of control systems for distributed parameter processes.

The major emphasis was placed on creating the model based control system from normal process data; thus insuring that the required process model would be readily available in an industrial setting. Only in this way, would these new control system designs find their way into widespread use in practice.

(3) Computer-Aided Design Software

The design tools resulting from each of the research projects were included in user friendly computer-aided design software available to the University and Industrial Community. In this way the results of our research were easily tested against current methods and brought more quickly into practical use.

Scientific and Technical Content

Industrial users consume approximately one-fourth of the total energy used in the United States today (more than 3 million barrels/day of oil equivalent). It is estimated that more than a third of this energy is unrecovered and thus lost. Though some of these losses are unavoidable, the incentives for more efficient process design and operation are significant. We cite a few examples typical for the process industries.

- If one third of this lost energy were to be conserved (1 million barrels/day), it would reduce the import cost of oil and balance of payments of the U.S. by more than $5 billion dollars/year at current prices.
- If ten percent of the energy in distillation separation processes in the U.S. could be conserved, the savings in fuel would amount to the equivalent of nearly 100,000 barrels/day of oil. This amounts to a dollar savings in imports of about 500 million dollars/year at current prices.
- Low conversion per pass and byproduct formation in chemical reactors are estimated to waste millions of barrels of oil per year through inefficient raw material usage and the requirement for energy intensive separation trains, such as distillation.
- Contraction in plant production rates in the Process Industry has resulted in reduced energy efficiency for old plants and limited plans for new plants. This means that there are strong incentives to develop new designs and plant revamps to allow efficient operation over a wide range of production rates.
- Recent assessments from industry indicate that very attractive returns on engineering manpower investment have resulted from process modification directed towards energy conservation.
- A detailed survey of processes at the DuPont Company resulted in the prediction that $500 million per year could be saved in manufacturing costs by the application of improved process control methods. These benefits would arise from both energy savings and improved productivity.

Thus research investments in improved process design and control hold the promise of high return in terms of energy savings.

A second crucial goal of process design and control research is to allow efficient production of uniform, high quality product. Because of worldwide availability of turn-key plants with state-of-the-art technology for many products, low wage rates in "off-shore" industry, and the low cost of raw materials and energy in some parts of the world, there are an increasing number of commodity chemicals and plastics that cannot be competitively produced in the U.S. with current technology and operating practice. Furthermore, the more static the technology in a given area, the more rapidly off-shore industry will be able to "catch-up" and erode our market position. Examples of problem areas in the U.S. chemical economy include methanol, olefins such as ethylene and propylene, commodity grade fibers such as nylons and polyesters, etc.

The best hope to reverse this deterioration in the competitive position of the U.S. process industry is to improve the methodology for developing process designs and process control schemes so as to make U.S. plants the most "high-tech" in the world. This means that our plants will have to

- be the most flexible and efficient to allow profitable operation over a wide range of production rates, and product specifications
- have the best product quality monitoring and control schemes to yield the highest quality product in the world
- be the most resilient to component failures and alarms situations so that absolute minimal off-spec. operation and down time is achieved
- be the most highly optimized for both steady state and transient operation (e.g.; continuous or batch, under steady state or product grade swings, etc.).

These are often conflicting requirements in process design and control so that optimal trade-offs are usually required. To achieve this, methodologies must be developed for obtaining good process understanding (i.e.; detailed models) from available information and for the application of this detailed knowledge in process design and control schemes. Furthermore, to have widespread impact, these ideas and techniques must be made available to the practicing engineer in a readily usable form.

Below we provide extensive lists of publications, short courses for industry, and seminars indicating how the research contributed to the solution of these problems.

Project Output

The results of the research carried out from June 1989 through November 2001 and supported by the Department of Energy have been reported in a series of research papers, conference presentations, short courses, and seminars. These are listed in detail below. Several additional papers are in preparation.

PUBLICATIONS AND PRESENTATIONS RESULTING FROM THE RESEARCH SINCE 1989

Research papers in referred journals

1. Ray, W. H. "Practical Benefits from Modelling Olefin Polymerization Reactors", **Transition Metal Catalyzed Polymerization: Ziegler-Natta Metathesis Polymerization**, Cambridge Univ. Press (1989).
2. Windes, L. C., Schwedock, M. J. and W. H. Ray. "Steady state and Dynamic Modelling of a Packed Bed Reactor for the Partial Oxidation of Methanol of Formaldehyde. I. Model Development." **Chem. Engr. Comm., Vol. 78**, 1-43 (1989).
3. Schwedock, J. J., Windes, L. C. and W. H. Ray. "Steady State and Dynamic Modelling of a Packed Bed Reactor for the Partial Oxidation of Methanol to Formaldehyde II. Experimental Results Compared with Model Predictions." **Chem. Engr. Comm., Vol. 78**, 45-71 (1989).
4. Congalidis, J. P., Richards, J. R. and W. H. Ray. "Feedforward and Feedback Control of a Solution Copolymerization Reactor." **AIChE Journal, Vol. 35**, 6, 891 (1989).

5. Ray, W. H. "Computer-Aided Design, Monitoring, and Control of Polymerization Processes". **1989 Berlin Workshop on Polymerization Reaction Engineering.**
6. Stevens, C. J. and W. H. Ray. "The Mathematical Modeling of Bulk and Solution Polymerization in a Tubular Reactor". ACS Symposium Series No. 404; **Computer Applications in Applied Polymer Science II: Automation, Modeling, and Simulation**, Chapter 28. American Chemical Society (1989).
7. Teymour, F. and W. H. Ray. "The Dynamic Behavior of Continuous Solution Polymerization Reactors - IV. Dynamic Stability and Bifurcation Analysis of an Experimental Reactor". **Chem. Eng. Sci., Vol. 44**, 9, 1967-1982 (1989).
8. Windes, L. C., Cinar, A. and W. H. Ray. "Dynamic Estimation of Temperature and Concentration Profiles in a Packed Bed Reactor". **Chem. Eng. Sci., Vol. 44**, 10, 2087-2106 (1989).
9. Sauer, B. B., Stock, R. S., Lim, K-H and W. H Ray. "Polymer Latex Particle Size Measurement Through High Speed Dielectric Spectroscopy". **J. of Applied Polymer Sci., Vol. 39**, 2419-2441 (1990).
10. Ray, W. H. "Polymerization Reaction Engineering" (invited review). **Proceedings of SLAP '91**, Guadalajara, Mexico (Oct. 1990).
11. Ray. W. H. "A New Mix of Skills for Process Control Engineers". **Control** P. 88 (June 1990).
12. Ray, W. H. "Modelling of Addition Polymerization Processes" (invited review). **Can. J. Ch.E. 69**, 626 (1991).
13. Yuan, H-G, Kalfas, G. and W. H. Ray. "Suspension Polymerization". J. **Macromolecular Science, C31**, 215 (1991).
14. Hutchinson, R. A. and W. H. Ray. "Polymerization of Olefins Through Heterogeneous Catalysis VIIa. The Effect of Condensation Cooling on Particle Ignition". **J. Appl. Poly. Sci. 43**, 1387 (1991).
15. Jerome, N. F. and W. H. Ray. "Control of Single Input-Single Output Systems with Time Delays and an Infinite Number of Right Half Plane Zeros". **Chem. Eng. Sci, 46**, 2003 (1991).
16. Jerome, N. F. and W. H. Ray. "Model-Predictive Control of Linear Multivariable Systems Having Time Delays and Right-Half Plane Zeros". **Chem. Eng. Sci., 47**, 4, 763-785 (1992).
17. Canu, P. and W. H. Ray. "Discrete Weighted Residual Methods Applied to Polymerization Reactions". **Computers in Chemical Eng., 15**, 549 (1991).
18. Scott, G. M., J. W. Shavlik, and W. H. Ray. "Refining PID Controllers Using Neural Networks". **Neural Computation, 4**, 746-757 (1992).
19. Teymour, F. and W. H. Ray. "Dynamic Behaviour of Continuous Polymerization Reactors - V. Experimental Investigation of Limit Cycle Behaviour for Vinyl Acetate Polymerization". **Chem. Eng. Sci., 47**, 15/16, 4121-4132 (1992).

20. Teymour, F. and W. H. Ray. "Dynamic Behaviour of Continuous Polymerization Reactors - VI. Complex Dynamics in Full Scale Reactors". **Chem. Eng. Sci., 47,** 15/16, 4133-4140 (1992).
21. Teymour, F. and W. H. Ray. "Chaos, Intermittency and Hysteresis in the Dynamic Model of Polymerization Reactor". **Chaos, Solitons and Fractals, 1,** 295 (1991).
22. Windes, L. C. and W. H. Ray. "A Control Scheme for Packed Bed Reactors Having a Changing Catalyst Activity Profile - I. On-Line Parameter Estimation and Feedback Control". **J. Process Control, 2,** 1, 23-42 (1992).
23. Windes, L. C. and W. H. Ray. "A Control Scheme for Packed Bed Reactors Having a Changing Catalyst Activity Profile - II. On-Line Optimizing Control". **J. Process Control, 2,** 1, 43-53 (1992).
24. Ray, W. H. "Modeling and Control of Polymerization Reactors". **Proceedings DYCORD-'92,** College Park, MD, April 1992.
25. Kaspar, M. H. and W. H. Ray. "Chemometric Methods for Process Monitoring and High-Performance Controller Design". **AIChE Journal, 38,** 10, 1593-1608 (1992).
26. Kaspar, M. H. and W. H. Ray. "Partial Least Squares Modelling as Successive Singular Value Decompositions". **Computers in Chem. Engng., 17,** 10, 985-989 (1993).
27. Kaspar, M. H. and W. H. Ray. "Dynamic PLS Modelling for Process Control". **Chem. Eng. Sci., 48,** 20, 3447-3461 (1993).
28. Scott, G. M. and W. H. Ray. "Creating Efficient Nonlinear Neural Network Process Models that Allow Model Interpretation". **J. Proc. Cont., 3,** 3, 163-178 (1993).
29. Scott, G. M. and W. H. Ray. "Experiences with Model-Based Controllers Based on Neural Network Process Models". **J. Proc. Cont. 3,** 3, 179-196 (1993).
30. Debling, J. A., G. C. Han, F. Kuijpers, J. VerBurg, J. Zacca, and W. H. Ray. "Dynamic Modeling of Product Grade Transitions for Olefin Polymerization Processes". **AIChE J., 40,** 3, 506-520 (1994).
31. Scott, G. M. and W. H. Ray. "Neural Network Process Models Based on Linear Model Structures". **Neural Computation, 6,** 718-738 (1994).
32. Pinto, J. C. and W. H. Ray. "The Dynamic Behavior of Continuous Solution Polymerization Reactors - VII. Experimental Study of A Copolymerization Reactor". **Chemical Engineering Science, 50,** 4, 715-736 (1995).
33. Pinto, J. C. and W. H. Ray. "The Dynamic Behavior of Continuous Solution Polymerization Reactors - VIII. A Full Bifurcation Analysis of A Lab-Scale Copolymerization Reactor". **Chemical Engineering Science, 50,** 6, 1041-1056 (1995).
34. Gay, David H. and W. H. Ray. "Identification and Control of Distributed Parameter Systems by Means of the Singular Value Decomposition". **Chemical Engineering Science, 50,** 10, 1519-1539 (1995).

35. Semino, Daniele and W. H. Ray. "Control of Systems Described by Population Balance Equations - I. Controllability Analysis". **Chemical Engineering Science, 50,** 11, 1805-1824 (1995).
36. Semino, Daniele and W. H. Ray. "Control of Systems Described by Population Balance Equations - II. Emulsion Polymerization with Constrained Control Action". **Chemical Engineering Science, 50,** 11, 1825-1839 (1995).
37. Zacca. J. J., S. X. Zhang, and W. H. Ray. "Reactor Runaway Phenomena in Polymerization Processes". In "International Symposium on Runaway Reactions and Pressure Relief Design", G. A. Melhem and H. G. Fisher, Ed., AIChE Press, 580-604 (1995).
38. Chakravarti, S., M. Marek, and W. H. Ray. "Reaction-diffusion system with Brusselator kinetics: Control of a quasiperiodic route to chaos". **Physical Review E, 52,** 3, 2407-2423 (1995).
39. Hyanek, I., J. Zacca, F. Teymour, and W. H. Ray. "Dynamics and Stability of Polymerization Process Flow Sheets". **I&EC Research, 34,** 11, 3872-3877 (1995).
40. Zacca, J. J., J. A. Debling, and W. H. Ray. "Reactor Residence Time Distribution Effects on the Multistage Polymerization of Olefins". **Proceedings 5th DECHEMA Workshop on Polymer Reaction Engineering,** Berlin (1995).
41. Saldívar, E. and W. H. Ray. "Detailed Modeling of Emulsion Copolymerization Processes". **Proceedings 5th DECHEMA Workshop on Polymer Reaction Engineering,** Berlin (1995).
42. Pinto, J. C. and W. H. Ray. "The Dynamic Behavior of Continuous Solution Polymerization Reactors - IX. Effects of Inhibition". **Chemical Engineering Science, 51,** 1, 63-79 (1996).
43. Ochs, S., P. Rosendorf, I. Hyanek, X. Zhang, and W. H. Ray. "Dynamic Flowsheet Modeling of Polymerization Processes Using POLYRED". **Computers Chem. Engng., 20,** 6/7, 657-663, 1996.
44. Zacca, Jorge J., J. A. Debling, and W. H. Ray. "Reactor Residence Time Distribution Effects on the Multistage Polymerization of Olefins - I. Basic Principles and Illustrative Examples, Polypropylene". **Chemical Engineering Science, 51,** 21, 4859-4886 (1996).
45. Zhang, Simon X., Nolan K. Read, and W. H. Ray. "Runaway Phenomena in Low Density Polyethylene Autoclave Reactors". **AIChE Journal 42,** 10, .2911-2924 (1996).
46. Read, N. K., S. X. Zhang, and W. H. Ray. "Simulations of a LDPE Reactor Using Computational Fluid Dynamics". **AIChE Journal, 43,** 1, 104-117 (1997).
47. Saldívar, E. and W. H. Ray. "Mathematical Modeling of Emulsion Copolymerization Reactors: Experimental Validation and Application to Complex Systems". **Industrial & Engineering Chemistry Research, 36,** 4, 1322-1336 (1997).
48. Zacca, J. J., J. A. Debling, and W. H. Ray. "Reactor Residence-Time Distribution Effects on the Multistage Polymerization of Olefins. Part

II. Polymer Properties - Bimodal Polypropylene and Linear Low Density Polyethylene". **Chemical Engineering Science, 52,** 12, 1941-1967 (1997).

49. Debling, J. A., J. J. Zacca and W. H. Ray. "Reactor Residence-Time Distribution Effects on the Multistage Polymerization of Olefins. Part III. Multi-layered Products - Impact Polypropylene". **Chemical Engineering Science, 52,** 12, 1969-2001 (1997).
50. Saldívar, E. and W. H. Ray. "Control of Semicontinuous Emulsion Copolymerization Reactors", **AIChE J. 43,** 8, 2021-2033 (1997).
51. Read, Nolan K. and W. H. Ray. "Application of Nonlinear Dynamic Analysis in the Identification and Control of Nonlinear Systems -- I. Simple Dynamics", **J. Process Control,** 8, 1, 1-15 (1998).
52. Read, Nolan K. and W. H. Ray. "Application of Nonlinear Dynamic Analysis in the Identification and Control of Nonlinear Systems -- II. More Complex Dynamics", **J. Process Control,** 8, 1, 17-34 (1998).
53. Read, Nolan K. and W. H. Ray. "Application of Nonlinear Dynamic Analysis in the Identification and Control of Nonlinear Systems -- III. *n*-Dimensional Systems", **J. Process Control,** 8, 1, 35-46 (1998).
54. Saldívar, Enrique, Petros Dafniotis, and W. H. Ray. "Mathematical Modeling of Emulsion Copolymerization Reactors I. Model Formulation and Application to Reactors Operating with Micellar Nucleation". **Journal of Macromolecular Science – Reviews in Macromolecular Chemistry & Physics, C38(2),** 207-325 (1998).
55. Villa, Carlos M., J. O. Dihora, and W. H. Ray. "Effects of Imperfect Mixing on Low-Density Polyethylene Reactor Dynamics". **AIChE Journal, 44,** 7, 1646-1656 (1998).
56. Ghielmi, Alessandro, Guiseppe Storti, Massimo Morbidelli, and W. H. Ray. "Molecular Weight Distribution in Emulsion Polymerization: Role of Active Chain Compartmentalization". **Macromolecules, 31,** 21, 7172-7186 (1998).
57. Chakravarti, Shrikar and W. H. Ray. "Boundary Identification and Control of Distributed Parameter Systems Using Singular Functions". **Chemical Engineering Science,** 54, 1181-1204 (1999).
58. Villa, C. M., B. L. Van Horn, and W. H. Ray. "Dynamics of Polymerization Reactors with Evaporative Cooling and Wall Heat Transfer". **Polymer Reaction Engineering, 7,** 2, 151-194 (1999).
59. Debling, Jon, S. D. Naik, and W. H. Ray. "A Fundamental Approach to Modeling Polyolefin Particle Morphology". **Preprint for SPE International Polyolefins Conference XI,** Houston, TX, Feb. 1999.
60. Takeda, Makoto and W. H. Ray. "Optimal-Grade Transition Strategies for Multistage Polyolefin Reactors". **AIChE Journal, 45,** 8, 1776-1793 (1999).
61. Villa, Carlos M. and W. H. Ray. "Nonlinear Dynamics Found in Polymerization Processes – A Review". **Chemical Engineering Science, 55,** 2, 275-290 (1999).

62. Kosek, Juraj and W. H. Ray. "Dynamics and Stability of Slurry Olefin Polymerization Processes". **Récents Progrès en Génie des Procédés,** 13, 97-104 (1999).
63. Gorbach, Andreas, S. D. Naik, and W. H. Ray. "Dynamics and Stability Analysis of Solid Catalyzed Gas Phase Polymerization of Olefins in Continuous Stirred Bed Reactors". **Chemical Engineering Science,** 55, 4461-4479 (2000).
64. Naik, Sanjeev D. and W. H. Ray. "Particle Morphology for Polyolefins Synthesized with Supported Metallocene Catalysts". **Journal of Applied Polymer Science, 79,** 14, 2565-2579 (2001).
65. Yao, Zhen and W. H. Ray. "Modeling and Analysis of New Processes for Polyester and Nylon Production". **AIChE Journal,** 47, 401-412 (2001).
66. Wells, Gary J. and W. H. Ray. "The Effects of Catalyst Activity Profiles on Olefin Polymerization Reactor dynamics in Slurry Loop and Tank Reactors". (Submitted to **AIChE Journal**).
67. Solórzano, Manuel Z. and W. H. Ray. "Dynamic Behavior of Chemical Reactors with Evaporative Cooling". (Submitted to **Chemical Engineering Science**).
68. Solórzano, Manuel Z. and W. H. Ray. "Dynamic Behavior of Reactors with Evaporative Cooling and Vapor Phase Dynamics". (Submitted **to Chemical Engineering Science**).
69. Solórzano, Manuel Z. and W. H. Ray. "Dynamic Behavior of Polybutadiene Reactors with Evaporative Cooling". (Submitted to **Chemical Engineering Science**).

- **Books**

Arkun, Y and W. H. Ray, ed's., "Chemical Process Control IV". AIChE Publications (1991).

A new book entitled, "Process Dynamics, Modeling, and Control" (co-authored with B. A. Ogunnaike), was published by Oxford University Press in November 1994. The sales have been good both in the university and in industry (DuPont ordered 800 copies for their control and plant operations engineers).

Short courses, conferences and workshops for Industry

1. "Polymerization Reaction Engineering", Transnational Training Project, Maastricht, Netherlands. A 5-day course in May 1989 for industrial participants from the U. S. and Europe. Lectured for one day. Other lecturers were from Canada, West Germany and East Germany.
2. "Olefin Polymerization", Novacor/Polystar Ltd., Calgary, Alberta, Canada. A 2-day course in July, 1989. Sole lecturer.
3. "Olefin Polymerization", Engineers India Ltd., New Delhi, India. A one-day workshop in December 1989 for industrial R & D staff and Indian professors as part of my duties as a UNIDO consultant to India.

4. Three 1 1/2 day Research Conferences were held at the Wisconsin Center for industrial supporters of our University of Wisconsin Polymerization Reaction Engineering Laboratory (UWPREL). Some 30 people from 12 sponsoring companies attended each annual conference in June 1989-2001
5. In November, 1994 a 6-hour short course on Polymerization Process Dynamics was given for about 30 engineers from industry; University of Eindhoven, Netherlands.
6. In February 1995, a Workshop on Process Control was put on for about 30 engineers from industry, part of continuing education program of South Texas Section of AIChE.
7. In November 1996, a two-day short course on "Olefin Polymerization" was put on for about 30 chemists and engineers at Nova Chemicals, Ltd., Calgary, Alberta, Canada.
8. In April 1998, a short course on Polymerization Processes was put on for about 100 engineers from industry, at the DSM Research labs, Geleen, Netherlands
9. In February 2001, a short course on computer-aided simulation and analysis of polymerization processes was put on at the Exxon Polymer Research Center, Baytown, TX.

Papers presented at technical meetings

1. Invited lecture: "Progress in Olefin Polymerization". ACS National Meeting, Dallas, April 1989.
2. Invited lecture: "Complex Dynamics and Chaos in Continuous and Semibatch Polymerization Processes". 7th Symposium on Energy Engineering Sciences, Argonne National Lab, June 1989.
3. Invited survey lecture: "Computer-Aided Design, Modelling, and Control of Polymerization Processes". Third International Workshop on Polymer Reaction Engineering, Berlin, FRG, Sept. 1989.
4. Gay, D. H. and W. H. Ray. "Applications of SVD for Modelling and Control of Distributed Parameter Systems". 1989 Annual Meeting of AIChE, San Francisco.
5. Teymour, F. and W. H. Ray. "Improved Operation of a Semibatch Polymerization Reactor Using Flowrate Scheduling". 1989 Annual Meeting of AIChE, San Francisco.
6. Sauer, B. B., Stock, R. S., Lim, K. H. and W. H. Ray. "Latex Particle Size Measurement Through High Speed Dielectric Spectroscopy". 1989 Annual Meeting of AIChE, San Francisco.
7. Invited lecture: "Complex Dynamics and Stability of Polymerization Reactors". All Czechoslovakia Meeting on Mathematical Modelling, Tatra Mountains, Czechoslovakia, Sept., 1990.
8. Invited Lecture: "Polymerization Reactor Modelling". Latin American Symposium on Polymers, Guadalajara, Mexico, Oct., 1990.

9. Pinto, J. C. and W. H. Ray. "Dynamics and Stability of Solution Copolymerization Reactors". 1990 Annual Meeting of AIChE, Chicago.
10. Smith, R. E. and W. H. Ray. "CONSYDEX - An Expert System for Automated Computer-aided Control System Design". 1990 Annual Meeting of AIChE, Chicago.
11. Ramanathan, S., et. al. "POLYRED - A CAD Package for Polymerization Processes." 1990 Annual Meeting of AIChE, Chicago.
12. Ray, W. H. Invited lecture: "Dynamic Behavior of Polymerization Reactors". Engineering Foundation Conference on Polymer Reaction Engineering, Santa Barbara, CA, March 1991.
13. Ramanathan and W. H. Ray. Invited lecture: "The Dynamic Behaviour of Polymerization Process Flowsheets". Engineering Foundation Conference on Polymer Reaction Engineering, Santa Barbara, CA, March 1991.
14. Ray, W. H. Invited lecture: "Modelling of Gas Phase Olefin Polymerization Reactors". Atlanta ACS Meeting, April 1991.
15. Ray, W. H. Invited lecture: "Modelling of Polymerization Processes". Simulation Sciences User Conference, Newport Beach, CA, October 1991.

15. Ray, W. H. Invited lecture: "Modelling of Polymerization Processes". Simulation Sciences User Conference, Newport Beach, CA, October 1991.

16. Kaspar, M. H. and W. H. Ray. "Chemometric Methods for Process Monitoring and High Performance Controller Design". 1991 Annual Meeting of AIChE, Los Angeles.
17. Pinto, J. C. and W. H. Ray. "Dynamics of Solution Copolymerization Reactors - Effects of Feed Impurities". 1991 Annual Meeting of AIChE, Los Angeles.
18. Kalfas, G., Yuan, H-G, and W. H. Ray. "Studies in Batch and Continuous Suspension Polymerization Processes". 1991 Annual Meeting of AIChE, Los Angeles.
19. Scott, G. M., Shavlik, J. W. and W. H. Ray. "Refining PID Controllers Using Neural Networks". NIPS Meeting, Denver, CO, December 1991.
20. Read, N. and W. H. Ray. "Application of Nonlinear Dynamic Analysis in the Identification and Control of Nonlinear Systems." 1992 annual meeting AIChE, Miami.
21. Adebekun, K., M. Estler, A. Galimidi, and W. H. Ray. "State Estimation for Monitoring Processes with Delayed Measurements". 1992 annual meeting AIChE, Miami.
22. Ray, W. H. "Modeling and Control of Polymerization Reactors". Proceedings DYCORD-'92, College Park, MD, April 1992.
23. Appert, T., L. Jacobsen, and W. H. Ray. "A General Framework for Modeling Polycondensation Processes". DECHEMA (1992).
24. Invited lecture, Engineering Foundation Conference on Chemical Reaction Engineering. "Dynamic Behavior of Polymerization Processes". St. Augustine, FL (Feb. 1994)

25. Hyanek, I., J. Zacca, F. Teymour, and W. H. Ray. "Dynamics and Stability of Polymerization Process Flowsheets Using POLYRED". Proceedings ADCHEM '94, Kyoto, Japan, May 1994.
26. Semino, D. and W. H. Ray. "Population Balance Control: Controllability Theory and Chemical Process Examples". Proceedings PSE '94, Kyonju, Korea, June 1994.
27. Scott, G. M. and W. H. Ray. "Using Knowledge-Based Neural Network Process Models for Model-Based Control". Proceedings ADCHEM '94, Kyoto, Japan, May 1994.
28. Zacca, J., I. Hyanek, and W. H. Ray. "Stability and Dynamics Behavior of Industrial Loop Reactors for Olefin Polymerization". 1994 Annual AIChE Meeting, San Francisco.
29. Hyanek, I., J. Zacca, and W. H. Ray. "Stability of Process Flowsheets Involving Chemical Reactors". 1994 Annual AIChE Meeting, San Francisco.
30. Smith, R. A. and W. H. Ray. "Automated Computer-Aided Design of Control Systems Through Artificial Intelligence". 1994 Annual AIChE Meeting, San Francisco.
31. Featured speaker, South Texas Section, AIChE, Houston, TX (February 1995). "Some Challenges in Polymerization Process Technology".
32. DOE Symposium on Energy Engineering Sciences, Argonne National Lab (March 1995). "Control of Complex Dynamics and Chaos in Distributed Parameter Systems", (with S. Chakravarti and M. Marek).
33. International Symposium on Runaway Reactors and Pressure Relief Design, Boston (August, 1995). "Reactor Runaway Phenomena in Polymerization Processes" (with J. Zacca and S. Zhang).
34. "Reactor Residence Time Distribution Effects on the Multistage Polymerization of Olefins" (with J. Zacca and J. Debling) at the 5th DECHEMA Workshop on Polymer Reaction Engineering, Berlin, Germany (October 1995).
35. "Detailed Modeling of Emulsion Copolymerization Processes", (with E. Saldívar) at the 5th DECHEMA Workshop on Polymer Reaction Engineering, Berlin, Germany (October 1995).
36. CAPE Platform of the Netherlands, Utrecht (October 1995). "Computer-Aided Design of Polymerization Processes".
37. "Modeling of Batch and Continuous Emulsion Copolymerization Reactors Operating Below the CMC" (with P. Dafniotis), 1995 Annual Meeting of AIChE, Miami (Nov. 1995).
38. "Control of Complex Dynamics and Chaos in Distributed Parameter Systems" (with S. Chakravarti), 1995 Annual Meeting of AIChE, Miami (Nov. 1995).
39. Invited paper at German University-Industry Kolloqium on Process Modeling - University of Stuttgart (October, 1996). "Modeling, Dynamics, and Control of Polymerization Processes".

40. Invited paper at Hyprotech World Technology Conference - San Antonio, TX (October 1996). "POLYRED - A Tool for Improved Design, Operation, and Control of Polymerization Processes".
41. "Critical Problems in Polymerization Process Dynamics", (invited paper in Symposium honoring Rutherford Aris), 1996 Annual Meeting of AIChE, Chicago (November, 1996).
42. "Modeling and Control of Polymerization Processes", (invited survey paper), 1996 Annual Meeting of AIChE, Chicago (November, 1996).
43. "Numerical Methods for Emulsion Copolymerization Reactor Models with Particle Aggregation", (with Petros Dafniotis), 1996 Annual Meeting of AIChE, Chicago (November, 1996).
44. American Control Conference, Albuquerque, NM (June 1997). "Boundary Identification and Control of Distributed Parameter Systems Using Singular Functions" (with Shrikar Chakravarti).
45. DECHEMA Statusseminar, "Nichtlineare Dynamik bei Chemischen Prozessen", Frankfurt, Germany (October, 1997). Keynote lecture" "Nonlinear Dynamics in Polymerization Processes".
46. "Effects of Imperfect Mixing on LDPE Reactor Dynamics when Ethylene Decompositon Reactions are Considered" (with Carlos Villa and Jitan Dihora), 1997 Annual Meeting of AIChE, Los Angeles (November 1997).
47. Keynote Lecture, SINTEF Research Conference, Trondheim, Norway (April 1998). "Polymerization Kinetics and Processes".
48. AMOCO Technical Conference, Naperville, IL (May 1998). "Polyolefin Processes and Future Trends".
49. DOE Technical Conference, Argonne, IL (May 1998). "Mixing Effects on the Dynamics of LDPE Reactors".
50. Keynote Lecture, CHISA Conference, Prague, Czech Republic (August 1998).

Papers presented at 1998 DECHEMA Workshop on Polymer Reaction Engineering, Berlin (October 1998):

51. "Morphological Development of Impact Polypropylene Produced in the Gas Phase with the $TiCl_4/MgCl_2$ Catalyst" (with Jon Debling).
52. "Role of Radical Compartmentalization in Chain Branching and Gel Formation in Emulsion Polymerization" (with A. Ghielimi, G. Storti,and M. Morbidelli).

Papers presented at 1998 Annual Meeting of AIChE, Miami (November 1998):

53. "Optimal Grade Transition Strategies for Multistage Olefin Polymerization Reactors" (with Mako Takeda).
54. "Dynamics of Polymerization Processes".
55. "Dynamics of Free-Radical Polymerization Reactors Having Both Evaporative and Wall Cooling" (with Carlos Villa and Brett VanHorn).
56. Invited Lecture, SPE Polyolefins Conference, Houston, TX (February 1999). "A Fundamental Approach to Modeling Polymer Particle Morphology".

57. Invited Lecture, National Medal of Science Symposium to honor Eli Ruckenstain, Buffalo, NY (June 1999). "Some Issues in Olefin Polymerization".
58. Conference on Controlled Polymer Synthesis, San Francisco, CA (Sept. 1999). "Modeling of RAFT Living Free-Radical Polymerization" (with Min Zhang).
59. ACS Conference on Polyolefins, Napa, CA (October 1999). "Kinetics of Bridged & Unbridged Metallocene Polyethylene Catalysts in Gas Phase and Slurry Phase Reactors" (with Shreyas Chakravarti).

Papers presented at 1999 Annual Meeting of AIChE, Dallas, TX (November 1999):

60. "Ethylene Copolymerization with Metallocene Catalysts in Gas Phase" (with Shreyas Chakravarti).
61. "Dynamic Behavior of CSTR's having Evaporative Cooling" (with Manuel Solórzano).
62. Engineering Foundation Conference on Polymer Reaction Engineering, Palm Coast, FL (March 2000). "Particle Thermal Stability for Supercritical Fluidized Beds", with Thor Mejdell, Shreyas Chakravarti, and Dennis Lo.
63. Plenary Lecture, International Symposium on Chemical Reaction Engineering (ISCRE 16), Cracow, Poland (September 2000). "Some Current Issues in Polymerization Reactor Design".
64. 2000 Annual Meeting of AIChE, Los Angeles, CA (November 2000). "Prediction of Morphology Development in Polymerization Induced Phase Separation and Growth", with Min Zhang.
65. Invited Lecture, ACS Polymillenial 2000 Conference, Kona, Hawaii (December 2000). "Give Your Catalyst a Good Home – How the Reactor Environment Influences Catalyst Performance".

Invited seminars describing work on the project

At Universities:

1989
- Department of Chemical Engineering, Lehigh University
- Department of Chemical Engineering, Israel Inst. Technology (TECHNION), Haifa, Israel - Special Lecture Series

1990
- Department of Chemical Engineering, University of Colorado
- Control Systems Group, University of Michigan

1991
- Department of Chemical Engineering, Cornell University
- Control Systems Group, University of California, Santa Barbara
- Applied Mathematics Center, Cornell University
- Department of Chemical Engineering, Rensselaer Polytechnic Institute
- Department of Chemical Engineering, Northwestern University

1992
- Dept. of Chemical Engineering, Princeton University
- Dept. of Chemical Engineering, Texas A & M University
- Control Systems Program, California Institute of Technology

- Dipartimento di Chimica Fissica Applicata, Politecnico di Milano, Italy
- Scuola Normale Superiore, Pisa, Italy

1993 • Peck Lecture at Illinois Institute of Technology
1994 • Dept. of Chemical Engineering, University of Toronto
- Kelly Lecture, Purdue University
- University of Amsterdam, Netherlands
- Dept. of Chemical Engineering, King Saud University, Riyadh, Saudi Arabia

1995 • Dept. of Chem. Engineering, State University of New York, Buffalo
- Dept. of Chemical Engineering, University of Minnesota
- Dept. of Chemical Engineering, University of Nebraska

1996 • Dept. of Chem Eng, University of Delaware, **Kurt Wohl Lecture**
1997 • Dept. of Chemical Engineering, Iowa State University
- Laboratorium für Technische Chemie, ETH Zürich
- Dept. of Chemical Engineering, Rice University

1998 • Dept. of Chemical Engineering, Kyoto University, Kyoto, Japan
- Dept. of Chemical Engineering, Tech. Univ. Norway, Trondheim
- **Roger Sargent Lecture**, Imperial College, London

1999 • Dept. of Chemical Engineering, University of Houston
2000 • Department of Chemical Engineering, Rutgers University
- Department of Chem Engi, University of Waterloo, Canada

At Industries:

1989 • Research and Development Department, Himont, Inc., Wilmington, DE
- Engineering Department, E. I. Dupont de Nemours & Co., Wilmington, DE
- Statoil Petrochemicals and Plastics, Bamble, Norway
- Research and Development Department, Bayer AG, Dormagen, Germany
- Process Technology Group, Novacor Chemicals, Ltd., Calgary, Alberta, Canada
- Baytown Polymers Center, Exxon Chemical Co., Baytown, TX (lecture series)
- Research and Development Quantum Chemical Co., Morris, IL
- Shell Development Co., Houston, TX
- High Tech Forum, 3M Company, St. Paul, MN
- DSM Research, Geleen, Netherlands (Lecture series)

1990 • Baytown Polymers Center, Exxon Chemical Co., Baytown, TX (lecture series)
- Elastomers Technology Dept., Uniroyal Chemical Co., Naugatuck, CT
- DSM Research, Geleen, Netherlands (lecture series)

- Hoechst A. G. Research, Frankfurt, Germany
- Ethyl Technical Center, Baton Rouge, LA

1991
- Elastomers Technology Department, Uniroyal Chemical Co., Naugatuck, CT
- Polymer Products Department, E. I. Dupont de Nemours & Co., Wilmington, DE
- BASF Research, Ludwigshaven, Germany
- DSM Research, Geleen, Netherlands
- Research and Development Dept., Union Carbide Corp., South Charleston, WV

1992
- Mobil Chemical Co., Edison, NJ
- Xerox Research Centre, Toronto, Ontario, Canada
- DSM Research, Geleen, Netherlands

1993
- DSM Research, Geleen, Netherlands

1994
- Mitsubishi Chemical Co., Kurashiki, Japan
- DuPont Research Lab, Geneva, Switzerland
- BASF Research, Ludwigshaven, Germany

1995
- BASF Research, Ludwigshaven, Germany
- DSM Research, Geleen, Netherlands

1996
- Bayer Research Laboratory - Leverkusen, Germany
- DSM Research Laboratory - Geleen, Netherlands
- Nova Chemicals, Ltd., Calgary, Canada

1997
- Research Labs of Hoechst AG, Frankfurt, Germany
- BASF Research, Ludwigshaven, Germany

1998
- Mitsubishi Chemical Research Labs, Mizushima, Japan
- Research Labs of Showa Denko, Japan
- Research Labs of Sumitomo Chemical, Chiba, Japan
- Goodyear Research Labs, Akron, OH

1999
- Research Labs of DuPont Dacron, Kinston, NC
- Research Labs of Union Carbide Polypropylene, Houston, TX
- Central Research Labs of DuPont, Wilmington, DE
- Exxon Polymer Research Center, Baytown, TX
- Goodyear Research Labs, Akron, OH

2000
- Technical Center, Chevron Chemical, Orange, TX
- Research Labs of Union Carbide Corp., Bound Brook, NJ