

Roger Sargent

## My Contribution to Broadening the Base of Chemical Engineering

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#### Abstract

This paper is a short account, from a personal viewpoint, of the various contributions I have made to expand the academic basis of chemical engineering from its origin in the unifying concept of unit operations, focussed on process design, to encompassing all the professional activities of industrial chemical engineers. This includes all aspects of planning and scheduling the operations as well as designing and controlling the process plant. The span of my career also happens to include the birth of the age of computing, with all the consequential implications.

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I, Roger William Herbert Sargent, was born on October 14, 1926, in Bedford, England. I won a scholarship to attend Bedford School, a well-known English public school, and then went to Imperial College in 1944 to study for a BSc degree in chemical engineering.

It was wartime, the end of the period of V1 "flying bomb" raids on London. Professor Dudley Newitt, the head of the Department of Chemical Engineering, was one of a secret group of science and engineering professors committed to supporting the military services by use of their scientific expertise, so the departments of Imperial College were the site of various mysterious research projects designed to assist this activity. There was FIDO (Fog Investigation Dispersal Operation), a project to surround airfields with channels of burning vaporized petroleum which enabled the Spitfires to take off and land safely even in foggy weather. This was developed into strings of plastic fuel, which were easier to lay out and burnt more efficiently and steadily. Then there were the Mulberry Harbours, which played such a vital role in giving beach protection for the D-day landings, as well as PLUTO (Pipeline Under the Ocean), a project to lay pipelines on the seabed across the channel to supply fuel for invading forces, immune from the depredations of German U-boats on vulnerable cross-channel tankers. The famous bouncing bomb that caused such devastation in the dam-busting expeditions was also a product of these activities.

Thus, my undergraduate laboratory experiments were enlivened by these parallel activities, which also demonstrated a wider and unusual scope of the application of technology.

I stayed on to do research for a PhD, again under the supervision of Professor Newitt. He was interested in developing a mobile plant for generating oxygen in submarines or high-altitude aircraft, and his idea was to replace the carefully leveled bubble-cap plates of the traditional double-column by packed columns, which were less vulnerable to tilting of the columns. I succeeded in developing a single-column version, using air itself as a refrigerating fluid and a single packed column of Berl saddles made of wire-gauze, that produced oxygen of 95% purity in a column only five feet high. The project was also unusual in requiring close cooperation with research engineers from the British Oxygen Company, and I learned a wide range of construction techniques.

My first job was at a French company, Société Anonyme L'Air Liquide. This was a fascinating experience; France was recovering from a long period of occupation by Germany and was very short of middle managers owing to forced employment in Germany. It also had a very different tradition from England. French ingenieurs were the product of the elite grande écoles; they were highly trained in mathematics but had little experience of practical application. They were expected to gain this experience by practical training on the job after employment.

I was recruited along with four French ingenieurs, and because of my different background soon found myself leading a team and teaching them to apply their mathematics to practical application, armed with a collection of electromechanical calculators.

It happened that a nonexecutive director of L'Air Liquide was also a director of Machines Bull, which was formed to develop electronic computers. She was very keen to introduce the new electronic computers to improve the efficiency of L'Air Liquide's Accounting Service, which was based on traditional electromechanical punch-card machines. On hearing of my activities, she recruited my help in extending the application to engineering calculations, and I found myself, along with my team, packed off to learn the techniques of computer programming from the research engineers at Machines Bull. We then pioneered the application of these techniques to engineering problems.

Other large changes were occurring in the low-temperature industry. The discovery of oxygenbased steelmaking created a demand for large quantities of oxygen in contrast to the small-scale but widespread provision of oxygen for welding purposes. The result was a need to build plants on a tonnage-oxygen scale next to steel plants, which caused an evolution in plant construction techniques. The discovery by ICI (Imperial Chemical Industries Ltd.) of polyethylene also created a need to separate ethylene from refinery off-gases, again on a large scale. L'Air Liquide's design department therefore needed to change its construction techniques and expand its design activities to cover a much wider and more complex range of physical properties.

French ingenieurs were not normally specialized but rather were expected to turn their hand to everything. Thus, I found my design team was expected to help with the construction and commissioning of the plants they designed, and the result was that we gained a wide range of experience in traveling to sites throughout Europe. L'Air Liquide also had subsidiaries in Canada, America, and Japan, so this travel also extended throughout the world.

After seven busy years, my wife unfortunately contracted polio, and I was suddenly faced with looking after two sons, ages two and three, essentially single-handed. L'Air Liquide provided me with liberal support to enable me to continue some part-time activity for my design group, but the experience revealed our vulnerability to isolation from our family, so we decided to return to England.

Naturally I consulted Professor Newitt on the possible openings, and he immediately offered me a Senior Lectureship to return to teach at Imperial College. I eventually yielded to his insistence and have had no regrets ever since.

At the time of my own degree course, chemical engineering was limited to the study of the chemistry and physics of large-scale continuous processes and dominated by the needs of the oil industry.

Computational techniques were primitive, as they were based mainly on graphical techniques, or at most successive approximation, and implemented by slide rule. Only steady-state operation could realistically be attempted, which put the emphasis on design rather than operation. Operation and control was considered a separate discipline with the target of simply achieving stable steady-state operation; units were represented by simple linear models.

The structure of a plant as a set of interlinked units had already given rise to the concept of "unit operations," and it was recognized that there were only a few basic types of processing, which could be studied independently. The recognition of the power of countercurrent operation of a sequence of units was also an important step that yielded particularly effective techniques for distillation, absorption, and heat exchange.

Professor Newitt delegated to me the control of the undergraduate course. We already had a well-developed small-group tutorial system to supplement lectures, and I was keen to broaden the techniques studied to include operation and control as well as to introduce the power of using a computer for calculations. I was also keen to extend the laboratory experiments to give the students an experience of running a pilot plant of realistic size with interacting units.

We constructed three pilot plants: a plant for separating carbon dioxide from air with a twincolumn using ethanolamine as solvent, a climbing film evaporator and fluidized-bed crystallizer with a rotary filter to separate the crystals, and a well-stirred batch reactor for a reversible reaction using either heating or cooling.

Of course, over the years we added more intensive instrumentation and facilities for modeling, simulating, and controlling the plants using our research tool SPEEDUP (Simulation Program for the Economic Evaluation and Design of Unsteady Processes) and its successor gPROMS (general PROcess Modelling System).

The unit operations approach had established the idea of specialized subroutines written to calculate the steady-state behavior of each unit operation, but the methods of linking these subroutines to compute the behavior of the whole plant were left to the ingenuity of the individual designer. There was therefore an immediate need to make a more systematic study of these interlinking techniques, in particular to deal with recycle loops of process material, as described by Sargent & Westerberg (1). Improvement of numerical techniques with the impact of computers gave rise to further developments, for example, those summed up in the textbook by Mah (2).

The choice of the units and their interlinkage is very much part of the design, a special aspect of the problem that has come to be called process synthesis. The earliest person to tackle the problem was D.F. Rudd (2a), but Ignacio Grossmann and I (3) pioneered a systematic attack on this problem of selecting the optimal configuration of heat-exchanger networks using integer programming, which was later generalized to an arbitrary set of interlinked units by Grossmann and colleagues (4). More recently Grossmann has shown that the problem is more efficiently solved using mixed logic and integer programming (5). Simpler approaches were proposed by Jim Douglas (6), using guidance from economic considerations; by Bodo Linnhoff and colleagues (7), using guidance from thermodynamics and generalizing the concept of pinch technology; and by myself (8), using the purpose of the unit linkages to determine the structure. In addition, George Stephanopoulos (9) examined various aspects of the problem using the techniques of artificial intelligence.

An equally important need was improved techniques for fitting equations to experimental data on physical properties, and a major breakthrough was achieved by the discovery of the concept of group contribution theory [see Fredenslund et al. (10)]. This has been the mainstay of developments over the years, but recently it has been possible to use quantum mechanics to predict physical properties, see Kazantsev et al. (10a) and this has been so successful that even changes in crystal habit with processing conditions can be predicted.

To extend consideration to process control, control engineers had well-established techniques for designing stable steady-state feedback controls given a linear state-space model for the process. However, for practical application there is a need to estimate parameters in the model from measurements on the plant, and the Kalman filter was a real breakthrough in this area. Kalman (11) showed that there is a duality between linear models for feedback control and those for statistical estimation of parameters in the process control model from process measurements, thus providing a practical tool for effective control.

The corrections tend to zero as the number of measurements increases, and this has resulted in much activity in self-tuning regulators, which has led to model-predictive control, thus providing a balance between model accuracy and maintaining effective control. Eric Ydstie (12, 12a) finally solved the problem of an optimal limited memory self-tuning filter.

Chemical processes are inherently nonlinear and subject to significant variations in feed conditions. Coping with the variation of feed conditions on a slower timescale required the study of dynamic behavior, which in turn required a significant improvement in numerical techniques for integration of differential equations; see, for example, Sargent (13) and the later refinements by Morison & Sargent (14). In addition, there arises a new need to cope with mixed systems of differential and algebraic equations, as first pointed out by Mah et al. (15). Much later this problem was addressed in general terms by Gritsis et al. (16).

Extending considerations from merely feasible design and optimization to optimal design and operation was also an important step [see Sargent (17)] and a new orientation, but again this required a whole new range of numerical techniques for both steady-state and dynamic optimization.

Following the publication of the theoretical Pontryagin principle (18), which generated much activity in aerospace control, Pollard & Sargent (19) described an important advance in the provision of a general technique for optimal process control, and Vassiliadis and colleagues (20–21) eventually solved the problem of computing nonlinear optimal control of multistage systems. In the meantime, the dramatic development in this area was the announcement by Charlie Cutler and colleagues (22) of dynamic matrix control, a form of online optimal control using simple linear-quadratic models, which had widespread industrial success.

The shift to optimization also made the supremacy of continuous processing less obvious and made it attractive in many cases to consider batch processing and even the use of multipurpose plant. This in turn raises a new issue, that of the scheduling of a sequence of discrete operations, and yet another range of numerical techniques was developed for this application; see, for example, Kondili et al. (23) and Shah et al. (24). This led to techniques for the scheduling of a completely general set of resources; see Zhang & Sargent (25). Work on methods of steady-state design and process synthesis, including the optimal design and scheduling of multiproduct batch plants, is summarized in the textbook by Biegler et al. (26).

Concluding this survey, it is interesting to note that major reorientations of ideas are usually (but not entirely) made by academics; contributions by industrialists are usually concerned with refinements to make ideas more practically useful. However, these different viewpoints are mutually beneficial and equally important for progress.

Over the whole of my career at Imperial College, my own Process Systems Research Group has pioneered responses to these various demands, and needless to say the ideas have been constantly incorporated into the teaching of the undergraduate course.

So far I have concentrated on responding to demands for improved techniques for modeling, simulating, designing, operating, and controlling process plants. However, we have not been immune to the need for safe operation of plants, or to the requirement to consider wider demands owing to living on a planet with limited resources, and to more general social needs.

In 1978 a French newspaper ran a competition to identify the leading schools in Europe for the teaching of engineering. This article declared the chemical engineering course at Imperial College as the undisputed leader of the chemical engineering courses in Europe.

Over my career, I have supervised 51 PhD research students, recruiting them widely from contacts throughout the world, with the sole criterion of their potential as research students; they have come from 27 different countries, and I have been richly rewarded by the results. Many members of them have gone on to rewarding jobs in industry, but a large number have become academics with research students of their own, and many have achieved international reputations in their own right.

My students have assiduously kept track of my resulting academic "family tree," and on my retirement it extended to seven generations and totaled more than 700 members.

I particularly treasure a letter I received from Basil Joffe, a former research student who was awarded the prestigious Computing and Systems Technology Computing Practice Award of the American Institute of Chemical Engineers. In his acceptance speech he paid tribute to my inspiration as his research supervisor and asked for a show of hands of members of my family tree. More than half of the audience members put up their hands.

In 1988, responding to a government initiative, I won a national competition for an Interdisciplinary Research Center in Process Engineering comprising members of the Chemical Engineering and Electrical Engineering Departments at Imperial College and University College, London; the link provided a biochemical dimension, and the government provided substantial research support over 10 years. In effect, we created a new branch of chemical engineering termed "chemical process systems engineering." This was the only center from the competition to survive for the full ten years, and it is still going strong. It is now the strongest component of the Imperial Chemical Engineering Department, provides collaboration among various departments supporting "systems" ideas, has a thriving industrial consortium to promote industrial collaboration, and has a successful spin-off company that provides worldwide sales and support for gPROMS, the successor to SPEEDUP, which won the Royal Academy's prestigious MacRobert Award.

I was very proud when, in 2002, the Center received a Queen's Anniversary Prize for excellence in the field of process engineering, citing particularly success in promoting collaboration between industry and academia.

#### **EDITORS' NOTE**

The editors would like to point out that Professor Sargent is too modest about the impact of his academic family tree. At the present time this tree contains more than 1,000 members worldwide. They have become captains of industry and winners of industrial technology prizes such as The Queen's Award for Enterprise in the UK. Many members of Professor Sargent's academic family have become academics themselves, and more than 50 currently hold professorships worldwide, including at Imperial College London, University College London, University of Cambridge, TU Denmark, ETH Zurich, NTU Athens, Norwegian University of Science and Technology Trondheim, University of Istanbul, NTU Taiwan, McMaster University, University of Queensland, MIT, Princeton, Carnegie Mellon University, University of Minnesota, University of Wisconsin, UC Santa Barbara, UCLA, Georgia Institute of Technology, and many more. His academic family members have been internationally recognized for their scholarship, and many have been elected to learned societies, including the U.S. National Academy of Engineering and the UK Royal Academy of Engineering. In short, Professor Sargent's academic family tree is a Who's Who in process systems engineering worldwide and one of his greatest accomplishments.

#### **DISCLOSURE STATEMENT**

The author is not aware of any affiliations, memberships, funding, or financial holdings that might be perceived as affecting the objectivity of this review.

#### LITERATURE CITED

- Sargent RWH, Westerberg AW. 1964. SPEED-UP (Simulation Programme for the Economic Evaluation and Design of Unsteady-State Processes) in chemical engineering design. *Trans. IChemE.* 42:190–97
- 2. Mah RSH. 1990. Chemical Process Structures and Information Flows. Boston: Butterworths
- Rudd DF. 1968. The synthesis of system designs: I. Elementary decomposition theory. AIChE J. 14:343–49
- Grossmann IE, Sargent RWH. 1978. Optimum design of heat exchanger networks. Comput. Chem. Eng. 2(1):1–7
- Caballero JA, Odjo A, Grossmann IE. 2007. Flowsheet optimization with complex cost and size functions using process simulators. *AICbE* J. 53:2351–66
- Grossmann IE. 2002. Review of nonlinear mixed-integer and disjunctive programming techniques. Optim. Eng. 3:227–52
- 6. Douglas JM. 1988. The Conceptual Design of Processes. New York: McGraw-Hill. 601 pp.
- Linnhoff B, Flower JR. 1978. Syntheses of heat exchanger networks: 1. Systematic generation of energy optimal networks. AIChE J. 24(4):633–42
- Sargent RWH. 1998. A functional approach to process synthesis and its application to distillation systems. Comput. Chem. Eng. 22(1–2):31–45
- Stephanopoulos G. 1990. Artificial intelligence in process engineering—current state and future trends. Comput. Chem. Eng. 14(11):1259–70
- Fredenslund A, Jones RL, Prausnitz JM. 1975. Group-combination estimation of activity coefficients in nonideal liquid mixtures. *AIChE J*. 21:1086–99
- 10a. Kazantsev AV, Karamertzanis PG, Pantelides CC, Adjiman CS. 2010. Ab initio crystal structure prediction for flexible molecules. Proc. Eur. Symp. Comput. Aided Process Eng., 20th, Naples, pp. 817–22. Berlin/Heidelberg: Elsevier
- Kalman RE. 1960. A new approach to linear filtering and prediction problems. J. Basic Eng., Trans. ASME, Ser. D 82(1):35–45
- Ydstie BE, Co TB. 1985. Recursive estimation with adaptive divergence control. Proc. IEEE D Control Theory Appl. 132(3):124–30

- Hill JH, Ydstie BE. 2004. Adaptive control with selective memory. Int. J. Adapt. Control Signal Process. 18:571–87
- Sargent RWH. 1964. Le calcul des colonnes de distillation. L'etat stationnaire et le comportment dynamique. Genie Chim. 91:65–77
- Morison KR, Sargent RWH. 1986. Optimization of multistage processes described by differentialalgebraic equations. *Numerical Analysis: Proc. Inf. Integr. Methods Archit. Syst. Workshop, 4tb, Guanajuato, Mexico.* Lecture Notes in Mathematics 1230:86–102. Berlin: Springer-Verlag
- Mah RSH, Michaelson S, Sargent RWH. 1962. The dynamic behaviour of multi-component multi-stage systems. Numerical methods for the solution. *Chem. Eng. Sci.* 17:619–39
- Gritsis DM, Pantelides CC, Sargent RWH. 1988. The dynamic simulation of transient systems described by index-two differential-algebraic equations. In *Proc. Int. Symp. Proc. Syst. Eng.*, *3rd*, *Sydney, Australia*, pp. 132–40. Barton, ACT, Aust.: Inst. Eng., Aust.
- 17. Sargent RWH. 1967. Integrated design and optimization of processes. Chem. Eng. Prog. 3(9):71-78
- 18. Pontryagin LS, Boltyanski VG, Gamkrilidze GV, Mischinko E. 1962. *The Mathematical Theory of Optimal Processes*. New York: Interscience
- Pollard GP, Sargent RWH. 1970. Off-line computation of optimal controls for a plate distillation column. Automatica 6:59–76
- Vassiliadis VS, Sargent RWH, Pantelides CC. 1994. Solution of a class of multistage dynamic optimization problems. 1. Problems without path constraints. *Ind. Eng. Chem. Res.* 33(9):2111–22
- Vassiliadis VS, Sargent RWH, Pantelides CC. 1994. Solution of a class of multistage dynamic optimization problems. 2. Problems with path constraints. *Ind. Eng. Chem. Res.* 33(9):2123–33
- Vassiliadis VS, Pantelides CC, Sargent RWH. 1994. Optimization of discrete-charge batch reactors. Comput. Chem. Eng. 18(Suppl.):S415–19
- 22. Cutler CR, Ramaker BL. 1980. Dynamic matrix control: a computer control algorythm. Proc. Joint Autom. Control Conf., San Francisco, Pap. WP5-B
- Kondili E, Pantelides CC, Sargent RWH. 1993. A general algorithm for short-term scheduling of batch operations—I. MILP formulation. *Comput. Chem. Eng.* 17(2):211–27
- Shah N, Pantelides CC, Sargent RWH. 1993. A general algorithm for short-term scheduling of batch operations—II. Computational issues. *Comput. Chem. Eng.* 17(2):229–44
- Zhang X, Sargent RWH. 1994. The optimal operation of mixed production facilities—a general formulation and some approaches for the solution. *Proc. Int. Symp. Proc. Syst. Eng.*, 5th, Singapore, 1:171–78. Republished 1996 in Comput. Chem. Eng. 20(617):897–904
- Biegler LT, Grossmann IE, Westerberg AW. 1997. Systematic Methods of Chemical Process Design. Upper Saddle River, NJ: Prentice Hall PTR

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