

Process Systems Engineering – A Retrospective View with Questions for the Future

Roger Sargent*
Imperial College, London

Abstract

The paper reviews the development of Process Systems Engineering from a personal view-point, selecting concepts from the past which have given rise to new paradigms, and hence led to improved understanding or advances in solution techniques, but which either still pose unresolved problems or hold the promise of further developments.

1. Review

The systems engineering approach seems to have had its origins in the 1940's in the efforts to exploit the possibilities of the newly invented electronic digital computers, which held out the promise that, if a problem could be precisely formulated, then in principle an algorithm could be developed to solve it, and hence implemented and solved on a computer without the need for further human intervention or expertise.

It considered a complex system as a collection of interacting "units", whose behaviour was well understood, and concentrated on understanding the interactions between them.

In these early days, chemical engineering was often described as "systems engineering applied to the problems of the process industries", and it was certainly true that the concept of "unit operations" identified a limited set of basic operations used in a wide variety of processes, and made possible their systematic study, independent of the substances processed. This in turn led to a better understanding of these operations, and hence to the development of simple models, such as the "theoretical plate" or the "film theory" for heat and mass transfer, to predict the essence of their behaviour.

The recognition that mixtures could be separated into fractions containing an arbitrarily low level of impurities by use of a reflux stream in a multi-stage countercurrent system was also a typical "systems" idea.

Equally important was the representation of the process by a "flow-diagram" or "flow-sheet", showing how the units were interlinked, and the recognition that conservation of materials and energy provided sufficient means to determine the unit interactions. However these ideas were developed long before electronic computers, and the flow-sheet calculations had to be devised on a case by case basis.

With the advent of the computer, the immediate task was to replace the many elegant graphical solution procedures then in general use by numerical algorithms, and engineers were faced with the need to understand available general numerical techniques or develop new ones of their own. As the storage capacity of computers expanded, it was possible to store more and more of the programs and the data, much of

* E-mail: r.w.h.sargent@ps.ic.ac.uk

which was common to many different programs, and the need for more systematic classification and storage quickly emerged.

Once past this phase, interest turned towards more systematic organization of the flow-sheet calculations. Here the use of graph theory [1] revealed a technique for identifying the groups of units linked by recycle streams (the "strong components"), which therefore had to be computed together, indicating both a decomposition of the problem and appropriate candidates for iteration within the groups. When "sequential modular" flowsheeting programs, which used subroutines for the unit calculations, were replaced by "equation-based" programs, these same techniques could be used to exploit the structure of the resulting large sparse systems of equations.

Natural developments from the process flow-sheet were Ferencz Friedler's "P-graphs" [2] for representing process synthesis routes, the concept of "super-structures" [3], which incorporate a variety of options within a single flow-sheet, thus providing a rational (but limited) basis for process synthesis, and Bodo Linnhoff's representation of heat-exchanger networks, associated with his "pinch technology" [4] approach for analysing these networks and for wider applications.

In Computing Science, "object-oriented programming" represented the ultimate generalization of this basic idea, but in the effort to achieve generality perhaps too much was sacrificed. As the success of the equation-based approach illustrates, efficiency depends crucially on the choice of the "units", and it is not always convenient or efficient to deal with very black boxes.

Optimization quickly became a central guiding principle [5], eventually applied to design, planning, operation and control, and permeating the whole field. However its many ramifications really require a separate review of a more mathematical kind, which would carry me too far from the themes I wish to pursue here, though inevitably it will intrude at various points.

Analogous developments occurred in other branches of engineering. For example in control engineering the "units" were described by transfer functions, and block diagrams were used to represent how these were linked; Manfred Morari's "internal model control" block diagram structure [6] provided for example a unified representation and treatment of the model predictive control problem.

Use of the concept of "state", which originally formed the basis for the development of thermodynamics, caused a paradigm shift in control from an emphasis on the transformation of inputs into outputs to one on the evolution of the system state under the influence of the inputs, leading to the development of the Kalman filter [7] for recursive estimation of the current state and revealing the duality between the concepts of observability and controllability [8].

The state viewpoint also provided a link to differential equation theory, and the possibility of tackling control for nonlinear systems, with another paradigm shift to the viewpoint of optimal control [9]. For some years the consequential computing requirements meant that this could only be used off-line to generate optimal control policies, but eventually Dave Cutler launched his "Dynamic Matrix Control" [10], showing that simple linear models could be used to produce a discrete-time linear-quadratic on-line optimal controller – and proved his point by launching a company to market the approach with outstanding success. Since these early days the increasing speed of computers and improvements in numerical techniques for both state estimation

and optimal control have made possible on-line use of more sophisticated nonlinear models and more realistic objective functions [11,12], making this the most promising paradigm for the future.

Meanwhile control engineers have become more aware of the need for protection against undue sensitivity of the controller to modelling and prediction errors, and the H-infinity approach to "robust control" [13], based on a worst-case analysis, has done much to produce a unified viewpoint.

The robustness issue raises the whole question of how to deal with uncertainty, not only in control but in any situation where we need to predict the consequences in order to take appropriate action. Catering for a worst-case outcome is safe if it is really possible, but it is usually unnecessarily conservative, and it would be preferable to cater only for outcomes above a certain level of probability, and within this constraint take action to deal with the most likely outcome.

There has been much discussion on whether there really is such a thing as a random occurrence or whether we are dealing with chaotic responses (responses to such a complicated and far-reaching set of influences that they appear to be unpredictable). However prediction using probability distributions has served us well, and in the absence of predictions of such distributions from chaos theory, we must be content with distributions based on empirical observation, with some assurance from the "central limit theorem" that many independent influences tend to combine to give a Gaussian distribution.

For large uncertainties the computational requirements may still be too heavy a price to pay for the additional assurance obtained, and in some cases this is better obtained by use of a weighted objective function, based on a small number of postulated scenarios [14]. (Of course this can be interpreted as a crude way of generating an approximate distribution function).

In spite of advances through the use of "parametric programming" [15], one cannot pretend that the problem is satisfactorily resolved, but we have to be content with the tools currently at our disposal.

Process engineering has always had to cope with relatively complex, poorly understood processes, exhibiting essentially nonlinear behaviour. An early difficulty, which had to be dealt with before successful dynamic simulation, let alone optimal control, was possible, was the problem of numerical integration of what are now known as "stiff" systems—systems whose responses to input changes are a combination of responses of different parts of the system operating on very different time-scales [16].

Happily this was resolved [17], but the extreme form of this problem, the inclusion of components with instantaneous responses, gives rise to differential-algebraic systems [18], and no fully-proved technique for dealing with this has yet been published. One can take refuge in the fact that no physical processes are really instantaneous, and model them accordingly, but the severe stiffness problem persists, and the fact remains that the assumption of instantaneity is the simplest way of modelling many real processes.

A related question is the paradoxical behaviour of symplectic integration techniques [19,20], which broadly speaking allow one to maintain the constancy of invariants of the system (such as the conservation of energy) during the numerical integration. Intuitively one would expect this to improve the accuracy of the integration, which is indeed the case for extremely long time intervals, but these methods are usually inferior

to classical methods over time-intervals of practical interest---and the reasons for this are not at all apparent!

For partial differential equations, the use of finite elements rather than finite-difference approximations to derivatives can be viewed as a useful "systems" approach, again allowing the imposition of conservation laws over these elements, but again the symplectic paradox is a basic cause for concern. The question of the validity of the Navier-Stokes equation as a valid model for real fluids is still an open question, and our own failure to produce a satisfactory general modelling program for fluid dynamics [21] causes us to question the validity of the basic assumptions widely used in packages for computational fluid dynamics.

Other uses of the state concept have also proved to be fruitful. The "state-task network" [22] was another extension of the flow-sheet concept, which opened the way to a systematic treatment of a wide variety of batch-processing systems, and this "functional" view of processes can be applied to processes in general to suggest new approaches both to the synthesis of new processes [23] and to the modelling of a given process [24]. An example is Jim Douglas's "hierarchical design" technique [25], which is based on deciding on the inclusion of some unit or feature in a process, or the need to examine this issue more closely, on the basis of its contribution to the enhancement of some "utility-measure" of the value of the whole process.

The application of the idea to the automatic generation of a dynamic mathematical model from a purely qualitative description of the process opens new perspectives and deserves a little more discussion:

There is no such thing as a perfect model, and all that we can hope to do is predict the evolution of a limited set of properties of the system of interest with reasonable accuracy. We also hope that the model will not be too sensitive to the simplifications and approximations used.. However the vague adjectives in this statement need more precise definition:

The set of properties of interest will be clear enough to the user, and immediately determines a set of physical laws which might be involved in their determination (in addition to the conservation laws).. We must assume that these "laws", either fundamental or empirical, but acceptable as adequate for the purpose, can be provided, either specifically or by selection from a previously stored library.

It is then a well defined mathematical problem (programmable for the computer) to reduce these potential relations to a minimal set (or detect that they are incomplete), and to identify a minimal subset of variables from which all the properties of interest can be explicitly computed at any point of time or space using only algebraic equations.

This minimal set of variables defines the instantaneous state of the system, and their evolution is completely determined by the system inputs and the remaining equations in the minimal set. These will in general be a mixed set of partial differential, ordinary differential and algebraic equations.

Thus we have our mathematical model.

Of course the computer has no creative powers, and we are still relying on human knowledge and insight to provide the essential ingredients and make the appropriate selections for the purpose in hand, but this framework suggests a systematic way of storing these ingredients and providing the parts of the analysis which can be automated.

The idea is also capable of extension to make use of human insight to simplify the model thus formed. Consider for example a simple flash vessel for separating liquid and vapour:

If we are willing to assume instantaneous separation, there will be two zones in the vessel, one occupied by liquid and the other by vapour, each described by its own subset of the state variables, and linked only by relations at the common boundary. If we specify this assumption, or equivalently the fact that there are two distinct zones, the computer can make the corresponding decomposition of the mathematical model.

Instead we might assume that each fluid is distributed over the whole volume of the vessel, with the ratio of liquid to vapour varying with height and some empirical relation for the shear force per unit volume between the fluids at each point. Setting this force to zero yields our original model, but if we wish to determine the rate of separation we might instead treat the mixture as a single pseudo-fluid, with point values of its state variables determined by local averaging over the two fluids in a small volume around the point. This local "system" can again be modelled in the same way, implying a hierarchical modelling process. For example, if we are willing to consider a single bubble and ignore the influence of neighbouring bubbles, our shear-force parameter could be obtained using Stokes' Law. Of course this simple model could be successively refined, up to the limit of a finite element approximation of the two-fluid mixture.---but at the cost of a corresponding increase in the computational effort required.

Thus by providing qualitative information on possible simplifications we can control the complexity of the generated model or even generate several alternatives and choose between them on the basis of their impact on some utility-measure for the whole process model, as in the Douglas hierarchical design approach. An advantage is that the user is fully aware of the approximations used in compiling the model.

Clearly the idea is capable of further elaboration, and its implementation involves a host of subsidiary issues to be duly examined, but I have said enough to indicate the possibilities.

For a number of years process systems engineering was focused on the process itself, but process systems engineers have steadily widened the scope of their interests, first to wider aspects of process management, then to multi-site operations, and eventually to consideration of the whole supply chain. They have also expanded their interests to a wider range of processes, such as metallurgical and biochemical processes, delved deeper into the physico-chemical and biochemical foundations of the knowledge required for improving their models, and attempted to embrace sister technologies such as computational fluid dynamics [26] and even molecular dynamics [27].

As the scope of their investigations has expanded, process systems engineers have had to extend their interests to a wider range of relevant techniques. Computer Science had meanwhile produced techniques for encapsulating, storing and using qualitative knowledge, grandly termed "expert systems", which provided engineers with an entirely different way of using computers, eagerly pressed into use for such purposes as providing or checking the integrity of operating instructions or techniques for safety checking and analysis. "Qualitative modelling" systems were developed in an attempt to extend the scope of expert systems and avoid the heavy investment required for the traditional quantitative modelling systems.

The so-called "artificial intelligence" school bent their minds to developing a whole range of techniques intended to provide computers with the means of emulating human thought processes, using a range of analogies to biochemical or other natural processes [28]. These had immediate intuitive appeal, and some have been widely adopted. For example the "genetic" algorithm for optimization has become very popular and emulation of neural networks [29] has proved to be remarkably successful in improving on classical techniques for parameter and state estimation. Such successes should not be ignored, but I confess to a personal bias for use of techniques which can be justified by a more classical mathematical analysis.

Of course there continues to be progress in developing such techniques. Wavelet theory [30] has provided a powerful tool for the analysis of multi-scale processes and mathematical logic and graph theory have been applied in a variety of ways: Early use of fault-trees and event-trees to trace the root cause of faulty behaviour and the consequences of a particular failure were extended to the use of directed signal graphs (digraphs) for this purpose [31], methods were developed to check complicated operational procedures [32], and the use of logic in "disjunctive programming" provides a powerful supplement to integer programming techniques [33].

2. Conclusion

I have tried to review developments over the whole span of my career, but with such a broad canvas I have had to be selective, and therefore been unable to mention many other interesting and seminal ideas. I have chosen themes which have specially interested me, and still give me cause for concern or seem to point to further developments, rather than attempting the impossible task of a comprehensive review, giving due credit to every idea in the ever-increasing avalanche of new ideas over an ever-widening field.

As the scope of process systems engineering has widened, so it has become more diffuse, and it is more and more difficult to define its boundaries or identify an essential core of expertise. Many would say that it is unnecessary, or even unwise, to attempt to do so, but an area which cannot be adequately defined risks losing its appeal.

Nevertheless I hope that this necessarily cursory review has shown that there are still plenty of issues to address, and that there is an increasing range of techniques to do the job.

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