Operations Research

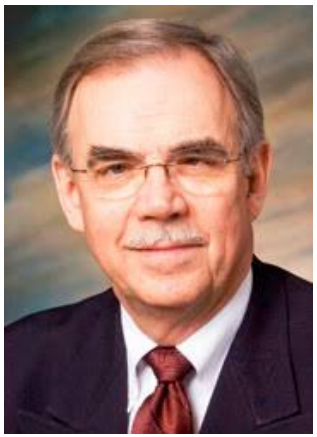
In Honor of Rex Reklaitis
2017 Recipient of the Warren K. Lewis Award

Ignacio E. Grossmann
Center of Advanced Process Decision-making
Department of Chemical Engineering
Carnegie Mellon University
Pittsburgh, PA, 15213

AIChE Annual Meeting
October 30, 2018

18AIChE Annual Meeting, Pittsburgh, PA

Gintaras (Rex) V. Reklaitis

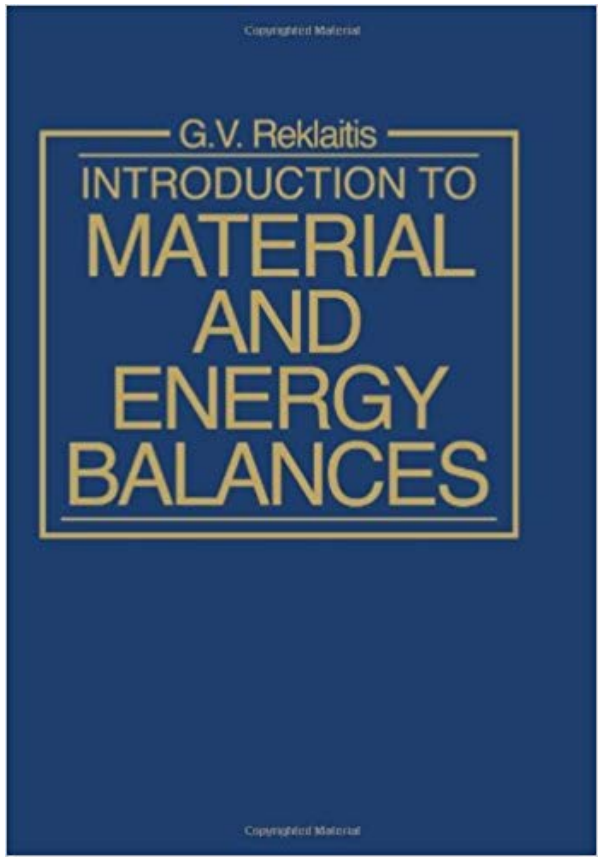


B.S., *IIT-Chicago* (1965)
M.S. and Ph.D., *Stanford* (1969)

NSF Postdoctoral Fellow: Institut für Operations Research, *ETH-Zürich*, Switzerland, 1969 - 1970.

Purdue University: Joined 1970
Assistant Dean Engineering, Grad. Education Research, 1985 - 1988
Edward W. Comings Distinguished Professor of
Head School Chemical Engineering (1987-2003)
Chemical Engineering, 2008–2010
Burton and Kathryn Gedge Distinguished Professor of
Chemical Engineering, 2010-present
Deputy Director, NSF ERC on Structured Organic Composites

Educational Contributions



Introduction to Material and Energy Balances

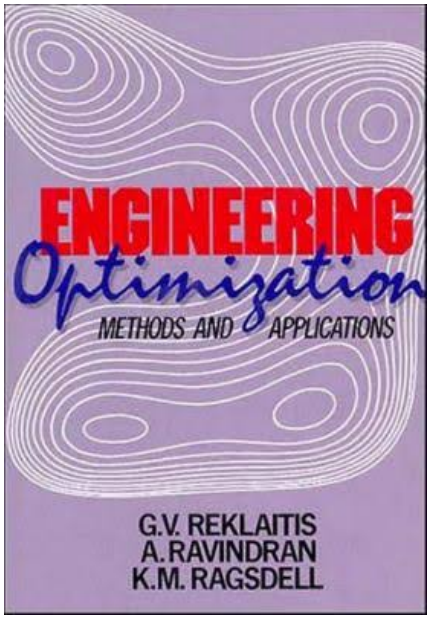
G.V. Rekalitis (1982)

Educational Contributions

Engineering Optimization: Methods and Applications

A. Ravindran, K. M. Ragsdell , G. V. Reklaitis

(Wiley, 1983, 2nd Edition, 2006)



Cited by 2193

Table Contents

Operations Research Topics

Trustee (since 1979) and President (1986-88) of CACHE

CACHE modules for Simulation of Industrial Processes
for the Undergraduate Laboratory.

Department Head Purdue (*1987-2003)*

Hired many faculty, built PSE area, Forney Hall

CAST Division of AIChE

Director, Chair of the Programming Board and Chair of the Division

Council for Chemical Research

Founded the International Committee

Major Contributions to Profession

Co-Founder of Area 10c: CAST Division of AIChE (1981)
Computers in Operations and Information Processing

1st International Conference on Foundations of Computer Aided Process Operations, July 5-10, 1987, Park City, Utah,

Editor-in-Chief and Co-Editor
Computers & Chemical Engineering (1986-2008)

Deputy Director, NSF Engineering Research Center on Structured Organic Particulate Systems, 7/ 2006; currently deputy director
PSE approach to Pharmaceutical Engineering

Research Contributions

Optimization

Uncertainty

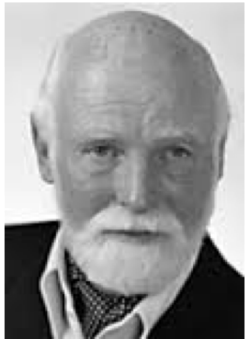
Scheduling

Batch Processing

Decomposition

Enterprise-wide Optimization

Optimization



Douglass J. Wilde

A COMPUTATIONALLY COMPACT SUFFICIENT CONDITION FOR CONSTRAINED MINIMA

G. Reklaitis and D. J. Wilde

Stanford University, Stanford, California

(Received July 25, 1967)

This paper derives a second-order sufficient condition in differential form for a local minimum of the nonconvex nonlinear programming problem under the requirement of twice continuous differentiability. The condition is complementary to the differential form of the Kuhn-Tucker necessary conditions and involves the positive definiteness of a matrix of constrained second derivatives of rank and order equal to the number of variables having vanishing first constrained derivatives. By using linear information, the condition avoids consideration of the entire second-order portion of the Taylor expansion of the Lagrangian. An example illustrating the test is included.

Operations Research 17, 425-436, (1969).

Geometric Programming via a Primal Auxiliary Problem*

$$\min f_0(x)$$

$$s.t.\ \ f_j(x) \le 1 \quad j \in J$$

$$f_j(x) = \sum_i c_i \prod_j x_j^{\alpha_{ij}} \quad j \in J$$

G. V. REKLAITIS
Purdue University
West Lafayette, Indiana 47907

D. J. WILDE
Stanford University
Stanford, California 94305

Abstract: This paper suggests the solution of geometric programs with degrees of difficulty by means of an auxiliary problem which is the reduced equivalent of the primal problem. The auxiliary problem is derived from the primal program by direct algebraic transformation and has a highly simplified convex separable structure. Using a condensation technique introduced by Duffin, it is shown that generalized polynomial programs can be solved via a sequence of approximating problems with a similar convex separable structure.

AIIE Transactions, 6:4, 308-317 (1974)

A Comparison of Computational Strategies for Geometric Programs[1]

P. V. L. N. SARMA,[2] X. M. MARTENS,[3] G. V. REKLAITIS,[4] AND M. J. RIJCKAERT[5]

Communicated by M. Avriel

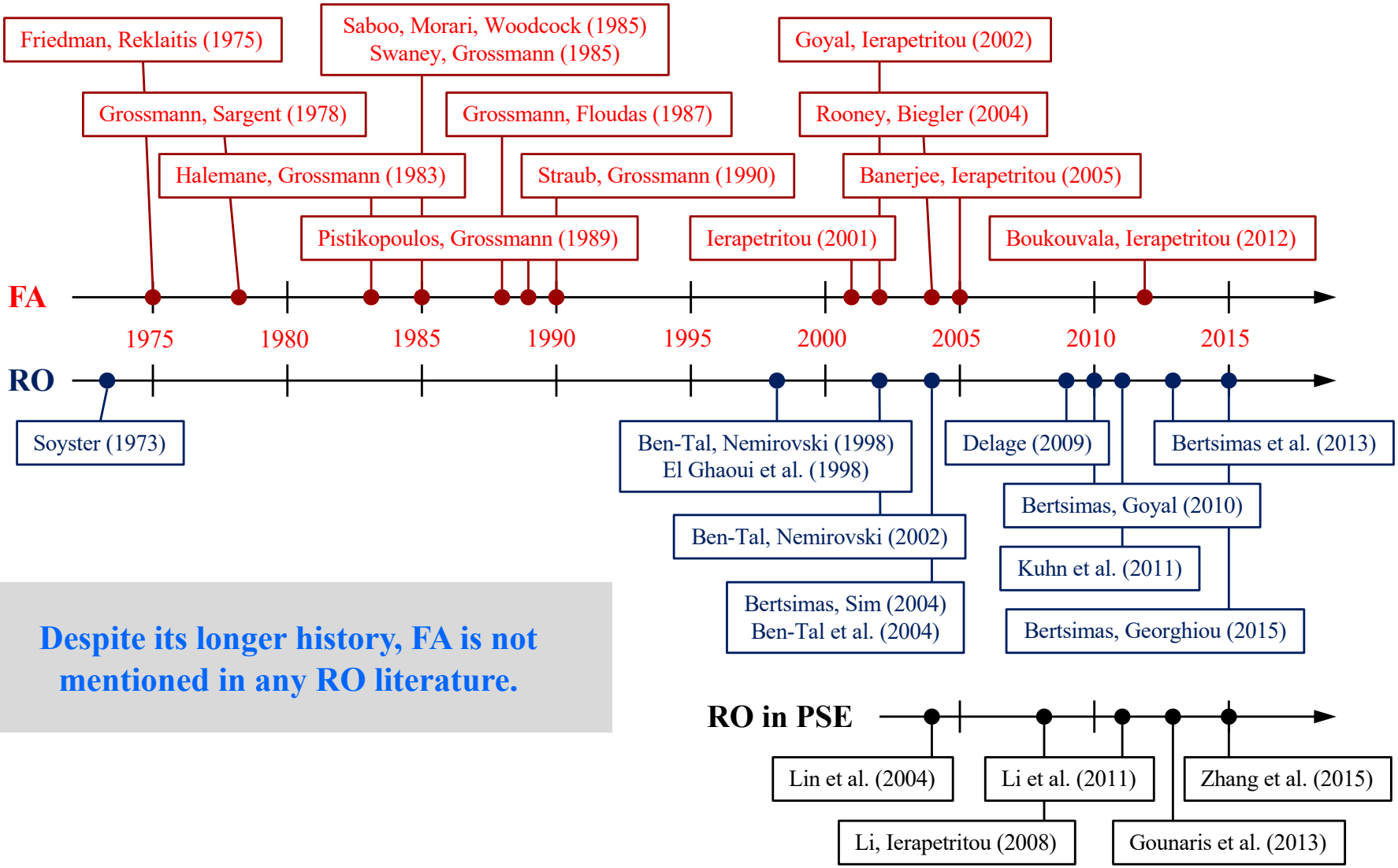
Abstract. Numerous algorithms for the solution of geometric programs have been reported in the literature. Nearly all are based on the use of conventional programming techniques specialized to exploit the characteristic structure of either the primal or the dual or a transformed primal problem. This paper attempts to elucidate, via computational comparisons, whether a primal, a dual, or a transformed primal solution approach is to be preferred.

Key Words. Nonlinear programming, geometric programming, computation, comparisons.

Journal of Optimization Theory and Applications, 26, No. 2, 1978.

Historical perspective Flexibility Analysis and Robust Optimization

Zhang, Lima, Grossmann, 2016)



Despite its longer history, FA is not mentioned in any RO literature.

Optimization under Uncertainty

Robust Optimization
Soyster (1973)

Flexible Solutions to Linear Programs under Uncertainty: Inequality Constraints

In most industrial applications the linear model used for optimization by linear programming involves significant uncertainties and inaccuracies in the model parameters. This paper presents a framework which allows uncertainties in the matrix elements of the linear program to be taken into account without requiring detailed knowledge of the statistical characteristics of these uncertainties. Three cases for the inequality constrained problem are considered: independent variations in the array elements, column dependent variations, and row dependent variations. In each case the problem can still be solved as a linear program. In the first two cases, the problem size is doubled, while for the row dependent case a finitely terminating cutting plane algorithm is constructed.

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AIChE J., 21, 77-83, (1975)

Flexible Solutions to Linear Programs under Uncertainty: Equality Constraints

This paper presents a framework which allows uncertainties in the matrix elements of an equality constrained linear program to be taken into account without requiring detailed knowledge of the statistical characteristics of these uncertainties. The results are derived using the model of the linear program with flexibility previously introduced for the inequality constrained case. However, because a feasible region common to all perturbed constraint sets does not exist in the equality constrained case, a flexibility set which intersects all perturbed sets individually rather than jointly is defined. The flexibility set is constructed by identifying a finite subset of all perturbed constraint sets which need to be investigated. Three cases for the equality constrained problem are considered: independent variations in the array elements, column dependent variations, and row dependent variations. In each case the problem is solved using a possibly large but decomposable linear program. In the first two cases, this program needs to be solved only once; while in the row dependent case an iterative but finite solution procedure is required.

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and
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West Lafayette, Indiana 47907

AIChE J., 21, 83-90, (1975).

Batch Scheduling

Reklaitis, G. V. Review of Scheduling of Process Operation. *AIChE Symp. Ser.* 78, 119-133 (1978).

Mauderli. A. M.: Rippin. D. W. T. Production Planning and Scheduling for Multipurpose Batch Chemical Plants. *Comp. Chem.Eng.* 3, 199 (1979).

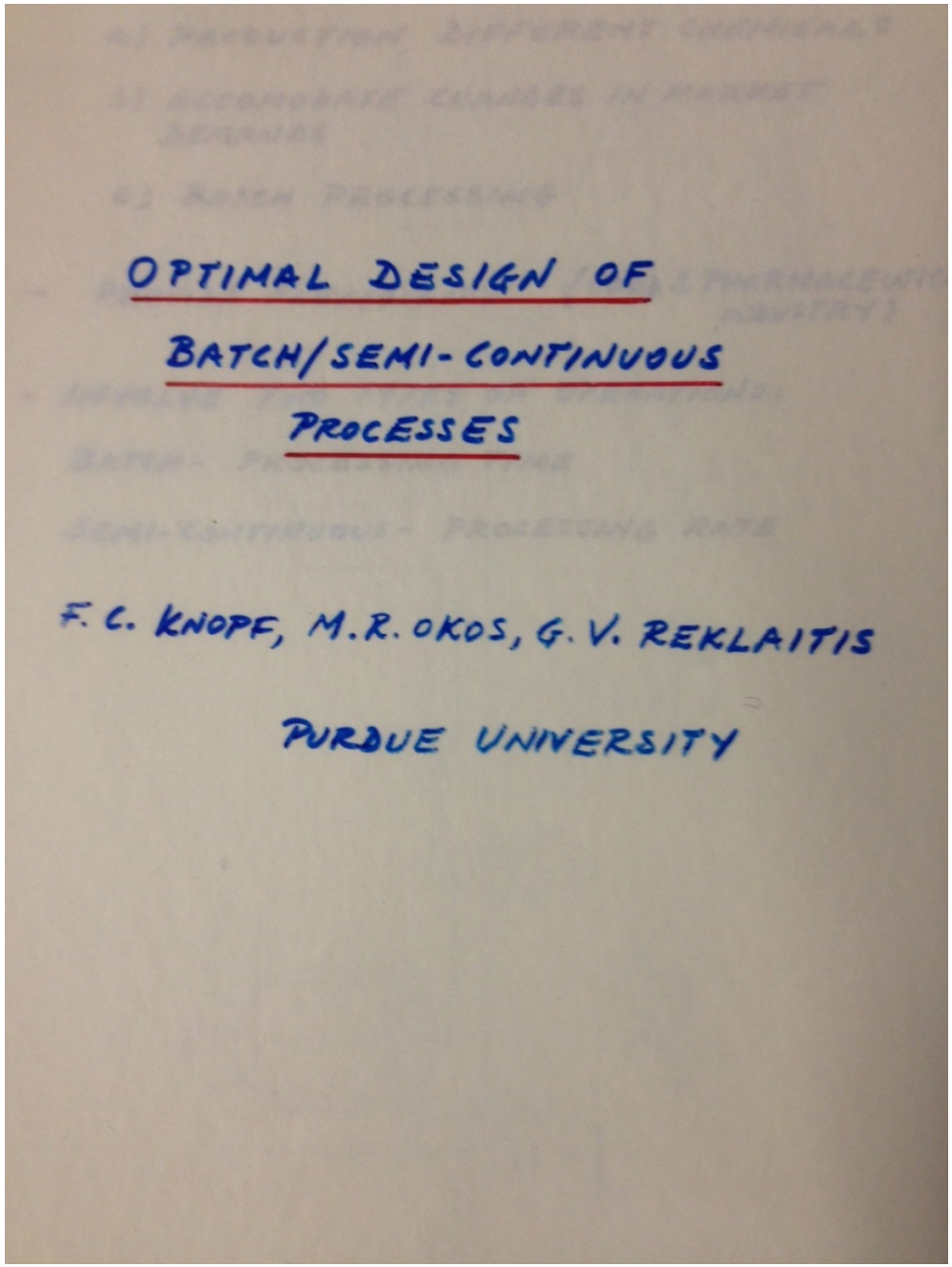
Optimal Design of Batch/Semicontinuous Processes

F. Carl Knopf, Martin R. Okos,* and Gintaras V. Reklaitis

School of Chemical Engineering and School of Agricultural Engineering, Purdue University, West Lafayette, Indiana 47907

A general formulation of the optimization problem arising in the design of plants involving batch/semicontinuous operations is presented. This extension of the minimum capital cost design problem properly accounts for the effects of semicontinuous units on the overall design. The continuous form of the general problem remains a geometric program and can be efficiently solved in the convexified form. A literature example solved using a generalized reduced gradient code is found to yield an improved design. The use of a total cost criterion and of empirical unit energy consumption correlations is suggested. An application study carried out with data derived from an operating cottage cheese process confirms the significance of the inclusion of energy costs in design optimization.

I&EC Process Design and Development, 21, 79 (1982).



I.E. Grossmann, CMU-PSE (CAD) Seminar (1983)

Optimal Design Batch Processes

Optimal Selection of Intermediate Storage Tank Capacity in a Periodic Batch/ Semicontinuous Process

Batch/semicontinuous chemical plants are usually designed either by assuming infinite intermediate storage or by assuming that the units themselves act as storage vessels, while the storage vessels are sized by rules of thumb or experience. In this paper, the case of an intermediate storage vessel which links one upstream batch/semicontinuous unit to one downstream batch/semicontinuous unit is analyzed. The units are assumed to operate with fixed cycle times and capacities. Expressions for determining the minimum storage tank capacity necessary to decouple the two units are derived from a mathematical model of the periodic process. Effects of the relative starting times of the two units on the required storage capacity are determined, thus suggesting the optimum process timings to minimize the same. Application of the results is illustrated by an example.

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G. V. REKLAITIS
Department of Chemical Engineering
Purdue University
West Lafayette, IN 47907

AIChE J., 29, 588, (1983).

SYNTHESIS AND SIZING OF BATCH/SEMICONTINUOUS PROCESSES: SINGLE PRODUCT PLANTS

N. C. YEH and G. V. REKLAITIS
School of Chemical Engineering, Purdue University, West Lafayette, IN 47907, U.S.A.

(*Received* 6 *February* 1987; *final revision received* 29 *May* 1987; *received for publication* 23 *June* 1987)

Abstract—An approach is reported for the preliminary design of single product batch/semicontinuous plants. The methodology consists of two components: a new approximate sizing procedure, which determines the number of units in parallel at each stage as well as the sizes of the batch and semicontinuous units and a set of synthesis rules, which serve to select structural features such as consecutive tasks that should be merged or split and tasks that should be separated by intermediate storage. The sizing procedure can accommodate both new plant design as well as some simple forms of retrofitting applications. The effectiveness of the approach is demonstrated with comparisons to designs obtained using nonlinear programming formulations solved by using a generalized reduced-gradient algorithm.

Computers & Chem. Engng., 11, 639-654, (1987)

Approaches to asynchronous decentralized decision making

I.P. Androulakis*, G.V. Reklaitis

School of Chemical Engineering, Purdue University, West Lafayette, IN 47907, USA

Received 11 February 1997; revised 22 September 1998; accepted 22 September 1998

Abstract

Motivated by the ideas of asynchronous relaxation algorithms this paper investigates optimal decision-making problems that exhibit decentralized characteristics. Such problems consist of a collection of interacting sub-systems, each one described by local properties and dynamics, joined together by the need to accomplish a common task which achieves overall optimal performance. Special properties of such systems that make them ideally suited for the framework of asynchronous computing are (a) the lack of a single overall objective describing the collective performance, and (b) the asynchronism in implementing topologically optimal decisions based on information which is local in space and time. A methodology for decentralized decision making is developed based on the solution of a series of sub-problems in which each minimizes a local objective while maximizing a common Lagrangian function, by generating independent approximations of an ascent direction in the space of the dual variables. The concepts are illustrated by means of motivating examples.

Computers & Chem. Engr, 23, 339-355(1999).

Optimization Supply Chain Level

Financial and financial engineering considerations in supply chain and product development pipeline management

J.M. Laínez[b], L. Puigjaner[b], G.V. Reklaitis[a,*]

[a] School of Chemical Engineering, Purdue University, West Lafayette, IN 47907-2100, United States
[b] Department of Chemical Engineering, Universitat Politècnica de Catalunya, Av. Diagonal 647, E08028 Barcelona, Spain

ARTICLE INFO

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Supply chain management
Product portfolio management
Supplier–customer relationships
Corporate value
Inventory management
Risk management
Flexibility

ABSTRACT

Enterprise-wide decision problems are receiving increasing attention in the process systems engineering literature. In particular, the supply chain and product development pipeline management components of this general class of problems have been subjects of intensive research in both their deterministic and their stochastic forms. The supply chain management (SCM) problem has seen work largely focused on the process operations and logistics components while for the product development pipeline management (PDPM) problem much of the attention has been on MILP formulations addressing the consequences of product failure during its development. In their full realization, both are recognized as challenging stochastic multi-stage decision problems. In this paper we discuss three important aspects of these problems that require further research: the realistic representation of the financial components and appropriate criteria for this class of problems, strategic management of supplier and customer relationships through inventory management and option contracts, and innovative approaches to suitably value and integrate a broader range of decisions available to management. We highlight and extend relevant contributions and case examples drawn from the recent literature that are emerging on these topics and use this work to point out further challenges.

Comput. & Chem Engr, 33, No. 12, 1999-2011 (2009)

Enterprise-wide modeling & optimization—An overview of emerging research challenges and opportunities

V.A. Varma, G.V. Reklaitis*, G.E. Blau, J.F. Pekny

School of Chemical Engineering, Purdue University, West Lafayette, IN, United States

Received 27 February 2006; received in revised form 13 November 2006; accepted 14 November 2006
Available online 16 January 2007

Abstract

The process systems engineering (PSE) as well as the operations research and management science (ORMS) literature has hitherto focused on disparate processes and functions within the enterprise. These themes have included upstream R&D pipeline management, planning and scheduling in batch and continuous manufacturing systems and more recently supply chain optimization under uncertainty. In reality, the modern process enterprise functions as a cohesive entity involving several degrees of cross-functional co-ordination across enterprise planning and process functions. The complex organizational structures underlying horizontally and vertically integrated process enterprises challenge our understanding of cross-functional co-ordination and its business impact. This article looks at the impact of enterprise-wide cross-functional coordination on enterprise performance, sustainability and growth prospects. Cross-functional coordination is defined as the integration of strategic and tactical decision-making processes involving the control of financial and inventory flows (both internal and external) as well as resource deployments. Initially, we demonstrate the existence of cross-functional decision-making dependencies using an enterprise network model. Subsequently, we discuss interactions between enterprise planning decisions involving project financing, debt-equity balancing, R&D portfolio selection, risk hedging with real derivative instruments, supply chain asset creation and marketing contracts which influence decision-making at the activity/process level. Several case studies are included to re-enforce the point that planning and process decisions need to be integrated.

Computers & Chem Engr, 32. pp. 692-711 (2007)

Recent Publications

Pharmacokinetic Based Design of Individualized Dosage Regimens Using a Bayesian Approach

José Miguel Laínez,*,† Gary Blau,† Linas Mockus,† Seza Orçun,‡ and Gintaras V. Reklaitis†

†School of Chemical Engineering, Purdue University, West Lafayette, Indiana 47907, United States

‡e-Enterprise Center, Discovery Park, Purdue University, West Lafayette, Indiana 47907, United States

ABSTRACT: Clinical trials and health care studies generate an enormous amount of data. This data is used by pharmaceutical companies during new drug development processes to characterize patient populations and determine a standardized dosage regimen for new patients, make commercial decisions, and gain approval from regulatory agencies. Nevertheless, the knowledge embedded in such data is rarely further exploited for customized patient care. In most cases, there is a significant difference between the pharmacokinetic profile of patients in a population, yet these differences are not reflected in the standardized dosage regimen. Here, a Bayesian methodology is proposed to individualize dosage regimens by combining the pharmacokinetic data collected from a patient population during clinical trials and additional data coming from a minimal number of serum samples from the new patient. In the Bayesian sense, the distribution of pharmacokinetic parameters from the population data is treated as prior information, and the posterior patient specific distribution of pharmacokinetic parameters is calculated. Then, such a posterior distribution is used to obtain dosage regimens that result in drug concentrations that are kept within the therapeutic window at a target confidence level for that patient. Moreover, a methodology is presented to suggest the sampling schedule for new patients so as to reduce the number of samples required to obtain well characterized individual pharmacometric parameters. Available pharmacokinetic data for Gabapentin, a therapeutic agent for epilepsy and neuropathic pain, is used to illustrate the concepts underlying the proposed strategy and the benefits of an individualized regimen over a standardized dosage regimen.

I&EC Research 50 (9) pp.5114-5130 (2011)

Recent Publications

Process systems engineering: From Solvay to modern bio- and nanotechnology. A history of development, successes and prospects for the future

George Stephanopoulos [a,*], Gintaras V. Reklaitis [b]

[a] Massachusetts Institute of Technology, 77 Massachusetts Avenue, Room 66-440, Cambridge, MA 02139, USA
[b] Purdue University, West Lafayette, IN 47907, USA

ARTICLE INFO

Article history:
Received 7 January 2011
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22 May 2011
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Available online 23 June 2011

Keywords:
Systems engineering
Process modeling
Process design
Process control
Process operations
Product design

ABSTRACT

The term Process Systems Engineering (PSE) is relatively recent. It was coined about 50 years ago at the outset of the modern era of computer-aided engineering. However, the engineering of processing systems is almost as old as the beginning of the chemical industry, around the first half of the 19th century. Initially, the practice of PSE was qualitative and informal, but as time went on it was formalized in progressively increasing degrees. Today, it is solidly founded on engineering sciences and an array of systems-theoretical methodologies and computer-aided tools. This paper is not a review of the theoretical and methodological contributions by various researchers in the area of PSE. Its primary objective is to provide an overview of the history of PSE, i.e. its origin and evolution; a brief illustration of its tremendous impact in the development of modern chemical industry; its state at the turn of the 21st century; and an outline of the role it can play in addressing the societal problems that we face today such as; securing sustainable production of energy, chemicals and materials for the human wellbeing, alternative energy sources, and improving the quality of life and of our living environment. PSE has expanded significantly beyond its original scope, the continuous and batch chemical processes and their associated process engineering problems. Today, PSE activities encompass the creative design, operation, and control of: biological systems (prokaryotic and eukaryotic cells); complex networks of chemical reactions; free or guided self-assembly processes; micro- and nano-scale processes; and systems that integrate engineered processes with processes driven by humans, legal and regulatory institutions. Through its emphasis on synthesis problems, PSE provides the dialectic complement to the analytical bent of chemical engineering science, thus establishing the healthy tension between synthesis and analysis, the foundation of any thriving discipline. As a consequence, throughout this paper PSE emerges as the foundational underpinning of modern chemical engineering; the one that ensures the discipline's cohesiveness in the years to come.

Chem Eng Sci 66, 4272-4306 (2011)

Recognition

AIChE Computing and Systems Technology Division, Computing in Chemical Engineering Award, 1984.

ASEE Chemical Engineering Division, Lectureship Award, 1994.

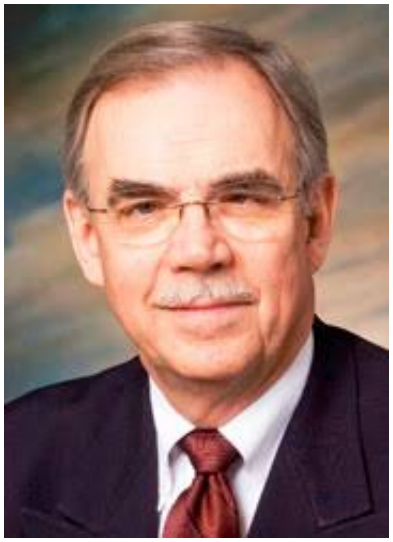
U.S. National Academy of Engineering, member, Feb 2007

Long Term Achievement Award in Computer Aided Process Engineering, European Federation of Chemical Engineering, 2013

Warren K. Lewis Award for Chemical Engineering Education, 2017

Summary

Rex Reklaitis



Pioneer and leader in Process Systems Engineering

- **Education:** ***Operations Research Methods***
- **Research:** ***Batch scheduling and design, Process Operations***

Many thanks for your contributions to PSE
Congratulations for 2017 Warren K. Lewis Award