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The (bio)chemical process industry is under an increasing pressure due to smaller margins and increasing societal and legislative demands for a sustainable future. In this context model-based optimization contributes to the solution because it serves to improve the processes’ performance.

A process simulator interface for multiobjective ...
Optimization of chemical processes solution manual pdf Optimization has found widespread use in chemical engineering applications, especially in the engineering of process systems. Problems in this domain often have many alternative solutions with complex economic and performance interactions, so it is

This book is an update of a successful first edition that has been extremely well received by the experts in the chemical process industries. The authors explain both the theory and the practice of optimization, with the focus on the techniques and software that offer the most potential for success and give reliable results. Applications and case studies in optimization are presented with new examples taken from the areas of microelectronics processing and molecular modeling. Ample references are cited for those who wish to explore the theoretical concepts in more detail.

Optimization is used to determine the most appropriate value of variables under given conditions. The primary focus of using optimisation techniques is to measure the maximum or minimum value of a function depending on the circumstances. This book discusses problem formulation and problem solving with the help of algorithms such as secant method, quasi-Newton method, linear programming and dynamic programming. It also explains important chemical processes such as fluid flow systems, heat exchangers, chemical reactors and distillation systems using solved examples. The book begins by explaining the fundamental concepts followed by an elucidation of various modern techniques including trust-region methods, Levenberg–Marquardt algorithms, stochastic optimization, simulated annealing and statistical optimization. It studies the multi-objective optimization technique and its applications in chemical engineering and also discusses the theory and applications of various optimization software tools including LINGO, MATLAB, MINITAB and GAMS.

In this book, optimization of chemical processes is performed using both classical and advanced algorithms.

This book addresses modern nonlinear programming (NLP) concepts and algorithms, especially as they apply to challenging applications in chemical process engineering. The author provides a firm grounding in fundamental NLP properties and algorithms, and relates them to real-world problem classes in process optimization, thus making the material understandable and useful to chemical engineers and experts in mathematical optimization.

Part I: Process design -- Introduction to design -- Process flowsheet development -- Utilities and energy efficient design -- Process simulation -- Instrumentation and process control -- Materials of construction -- Capital cost estimating -- Estimating revenues and production costs -- Economic evaluation of projects -- Safety and loss prevention -- General site considerations -- Optimization in design -- Part II: Plant design -- Equipment selection, specification and design -- Design of pressure vessels -- Design of reactors and mixers -- Separation of fluids -- Separation columns (distillation, absorption and extraction) -- Specification and design of solids-handling equipment -- Heat transfer equipment -- Transport and storage of fluids.

The Leading Integrated Chemical Process Design Guide: Now with New Problems, New Projects, and More More than ever, effective design is the focal point of sound chemical engineering. Analysis, Synthesis, and Design of Chemical Processes, Third Edition, presents design as a creative process that integrates both the big picture and the small details–and knows which to stress when, and why. Realistic from start to finish, this book moves readers beyond classroom exercises into open-ended, real-world process problem solving. The authors introduce integrated techniques for every facet of the discipline, from finance to operations, new plant design to existing process optimization. This fully updated Third Edition presents entirely new problems at the end of every chapter. It also adds extensive coverage of batch process design, including realistic examples of equipment sizing for batch sequencing; batch scheduling for multi-product plants; improving production via intermediate storage and parallel equipment; and new optimization techniques specifically for batch processes. Coverage includes Conceptualizing and analyzing chemical processes: flow diagrams, tracing, process conditions, and more Chemical process economics: analyzing capital and manufacturing costs, and predicting or assessing profitability Synthesizing and optimizing chemical processing: experience-based principles, BFD/PFD, simulations, and more Analyzing process performance via I/O models, performance curves, and other tools Process troubleshooting and "debottlenecking" Chemical engineering design and society: ethics, professionalism, health, safety, and new "green engineering" techniques Participating successfully in chemical engineering design teams Analysis, Synthesis, and Design of Chemical Processes, Third Edition, draws on nearly 35 years of innovative chemical engineering instruction at West Virginia University. It includes suggested curricula for both single-semester and year-long design courses; case studies and design projects with practical applications; and appendixes with current equipment cost data and preliminary design information for eleven chemical processes–including seven brand new to this edition.

Process models are always associated with uncertainty, due to either inaccurate model structure or inaccurate identification. If left unaccounted for, these uncertainties can significantly affect the model-based decision-making. This thesis addresses the problem of model-based optimization in the presence of uncertainties, especially due to model structure error. The optimal solution from standard optimization techniques is often associated with a certain degree of uncertainty and if the model-plant mismatch is very significant, this solution may have a significant bias with respect to the actual process optimum. Accordingly, in this thesis, we developed new strategies to reduce (1) the variability in the optimal solution and (2) the bias between the predicted and the true process optima. Robust optimization is a well-established methodology where the variability in optimization objective is considered explicitly in the cost function, leading to a solution that is robust to model uncertainties. However, the reported robust formulations have few limitations especially in the context of nonlinear models. The standard technique to quantify the effect of model uncertainties is based on the linearization of underlying model that may not be valid if the noise in measurements is quite high. To address this limitation, uncertainty descriptions based on the Bayes' Theorem are implemented in this work. Since for nonlinear models the resulting Bayesian uncertainty may have a non-standard form with no analytical solution, the propagation of this uncertainty onto the optimum may become computationally challenging using conventional Monte Carlo techniques. To this end, an approach based on Polynomial Chaos expansions is developed. It is shown in a simulated case study that this approach resulted in drastic reductions in the computational time when compared to a standard Monte Carlo sampling technique. The key advantage of PC expansions is that they provide analytical expressions for statistical moments even if the uncertainty in variables is non-standard. These expansions were also used to speed up the calculation of likelihood function within the Bayesian framework. Here, a methodology based on Multi-Resolution analysis is proposed to formulate the PC based approximated model with higher accuracy over the parameter space that is most likely based on the given measurements. For the second objective, i.e. reducing the bias between the predicted and true process optima, an iterative optimization algorithm is developed which progressively corrects the model for structural error as the algorithm proceeds towards the true process optimum. The standard technique is to calibrate the model at some initial operating conditions and, then, use this model to search for an optimal solution. Since the identification and optimization objectives are solved independently, when there is a mismatch between the process and the model, the parameter estimates cannot satisfy these two objectives simultaneously. To this end, in the proposed methodology, corrections are added to the model in such a way that the updated parameter estimates reduce the conflict between the identification and optimization objectives. Unlike the standard estimation technique that minimizes only the prediction error at a given set of operating conditions, the proposed algorithm also includes the differences between the predicted and measured gradients of the optimization objective and/or constraints in the estimation. In the initial version of the algorithm, the proposed correction is based on the linearization of model outputs. Then, in the second part, the correction is extended by using a quadratic approximation of the model, which, for the given case study, resulted in much faster convergence as compared to the earlier version. Finally, the methodologies mentioned above were combined to formulate a robust iterative optimization strategy that converges to the true process optimum with minimum variability in the search path. One of the major findings of this thesis is that the robust optimal solutions based on the Bayesian parametric uncertainty are much less conservative than their counterparts based on normally distributed parameters.

Many engineering, operations, and scientific applications include a mixture of discrete and continuous decision variables and nonlinear relationships involving the decision variables that have a pronounced effect on the set of feasible and optimal solutions. Mixed-integer nonlinear programming (MINLP) problems combine the numerical difficulties of handling nonlinear functions with the challenge of optimizing in the context of nonconvex functions and discrete variables. MINLP is one of the most flexible modeling paradigms available for optimization; but because its scope is so broad, in the most general cases it is hopelessly intractable. Nonetheless, an expanding body of researchers and practitioners — including chemical engineers, operations researchers, industrial engineers, mechanical engineers, economists, statisticians, computer scientists, operations managers, and mathematical programmers — are interested in solving large-scale MINLP instances.

Optimization problems abound in most fields of science, engineering, and tech nology. In many of these problems it is necessary to compute the global optimum (or a good approximation) of a multivariable function. The variables that define the function to be optimized can be continuous and/or discrete and, in addition, many times satisfy certain constraints. Global optimization problems belong to the complexity class of NP-hard prob lems. Such problems are very difficult to solve. Traditional descent optimization algorithms based on local information are not adequate for solving these problems. In most cases of practical interest the number of local optima increases, on the aver age, exponentially with the size of the problem (number of variables). Furthermore, most of the traditional approaches fail to escape from a local optimum in order to continue the search for the global solution. Global optimization has received a lot of attention in the past ten years, due to the success of new algorithms for solving large classes of problems from diverse areas such as engineering design and control, computational chemistry and biology, structural optimization, computer science, operations research, and economics. This book contains refereed invited papers presented at the conference on "State of the Art in Global Optimization: Computational Methods and Applications" held at Princeton University, April 28-30, 1995. The conference presented current re search on global optimization and related applications in science and engineering. The papers included in this book cover a wide spectrum of approaches for solving global optimization problems and applications.

A presentation of techniques in advanced process modelling, identification, prediction, and parameter estimation for the implementation and analysis of industrial systems. The authors cover applications for the identification of linear and non-linear systems, the design of generalized predictive controllers (GPCs), and the control of multivariable systems.