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Optimization

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I. INTRODUCTION

Optimization is the act of obtaining the best result possible or the effort for achieving the optimal solution under a given set of circumstances (1). In design, development, processing operation, and maintenance of engineering systems, common goals are either to minimize the cost or maximize the desired profits as product quality and operation yield. A systematic and efficient way to meet these goals is to place the emphasis on design and process optimization for manufacturability/performance (or yield), quality, and cost (2, 3). Such operations should be made efficient by applying the relevant optimization methods and taking the appropriate technological and managerial decisions among all possible alternatives.

Optimization can be defined as the process of finding the conditions that give the optimum (maximum or minimum) value of a function of certain decision variables subject to restrictions or constraints that are imposed (2). Optimization may be the process of maximizing a desired quantity or minimizing an undesired one. The conditions (values of the processing variables) that produce the desired optimum value are called *optimum conditions* while the best of all feasible designs is called *optimal design*. In its most general meaning, optimization is the effort and process of making a decision, a design, or a system as perfect, effective, or functional as possible.

Optimization for a system may mean the design of system parameters or the modification of its structure to minimize the total cost of the system's products under boundary conditions associated with available materials, financial resources, protection of the environment, and governmental regulation, taking into account the safety, operability, reliability, availability, and maintainability of the system. Optimizers or decision makers use optimization in the design of systems and processes, in the production and in systems operation. Some examples of the optimization use are: selection of processes or size of equipment, equipment items and their arrangement, operation conditions (temperature, pressure, flow rate, chemical composition of each stream in the system), equipment combination in specific processes to increase the overall system availability, etc.

Formal optimization theory encompasses the special methodology, techniques, and procedures used to decide on the one specific solution in a defined set of possible alternatives that will best satisfy a selected criterion or function. The application of scientific methods and techniques to decision-making problems based on mathematical programming techniques may achieve the optimum of the operation result—the maximization or minimization of the criterion or function.

A number of optimization methods have been developed for solving different types of optimization problems and hence various methods of efficient experimentation and simulation are available for performing the optimization. In many applications, the process to be optimized can be formulated as a mathematical model and the optimization experiments may be contacted or simulated in software. Today, even very large and complex systems can be modeled by means of computers, and optimization can yield substantially improved benefits.

Optimization methods have been found effective in many areas of engineering design and operation or even in business systems. In chemical processes, optimization methods were developed in an effort to produce high-quality products under normal manufacturing and working conditions, reducing their functional variations under real manufacturing circumstances (low quality of raw materials, poor manufacturing equipment, etc.) and further lowering the cost of making the product (including development and manufacturing). A wide variety of problems in the design, construction, operation, and analysis of chemical plants or industrial processes can be solved by optimization. These methods have particular economical and technological interest for food engineers, as they are widely used in food processes to achieve high efficiency in design, development and manufacturing. Now optimization methods are used routinely in industrial processes of foods.

In this chapter, an overview of the principles involved in design and process optimization is presented, the appropriate methods of optimization are described, and the applications of optimization in food engineering, especially in food extraction processing, are reviewed.

II. OPTIMIZATION THEORY

A. Quality Engineering—The Design Optimization Problem

The quality of a product or a manufacturing process can be quantified in terms of the deviation from the target performance due to undesirable effects by factors external to the product, manufacturing imperfection or deterioration/changing of product performance characteristics (3).

In a representative design optimization problem of a product or a process the common elements must be considered (Fig. 1). The response (y) is influenced by various factors; the dependence of the response y on the factors can be denoted by a function (f) or a mathematical model. Input or signal factors (or pre-assigned parameters) (s) are selected by the engineering knowledge and are set by the operator to attain the intended output (target performance). Control factors (or design or decision variables) (x) are the product or process parameters specification, and their best values (levels) are determined by the designer using a number of criteria. Noise factors (z) are the uncontrollable factors and their levels change from the environmental conditions of manufacture.

One approach to reduce the variation of a product or process is to limit or eliminate the noise factors. The role of design optimization is first to center the design parameters specifying the levels of control factors in order to minimize sensitivity to all noise factors. Product or process design can make the product or process robust against all factors, whereas manufacturing process design and actual manufacturing can reduce only the variation due to manufacturing imperfection.

A typical engineering problem can be posed as a process represented by some equations or by experimental data, while a performance criterion as minimum cost, maximum yield, etc. The process or model and the performance criterion comprise the optimization problem. The goal of optimization is to find

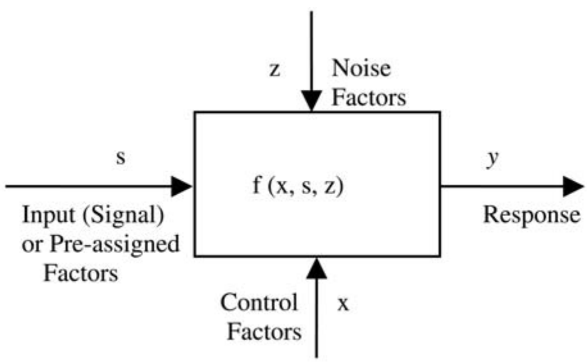

Figure 1 Block diagram of a product or a process in an optimization problem.

the values of the variables in the process that yield the best (maximum or minimum) value of the performance criterion while satisfying the constraints—this is the optimization of a given problem.

B. Classification of Design Problems

Design problems can be broadly classified into static and dynamic problems depending upon the absence or presence of signal factors, respectively (3). Static refer to problems in which the values of the dependent variables remain constant with respect to time, while dynamic problems represent the ones where the process-dependent variables change with time (2).

Static problems are also classified depending whether the response is continuous or discrete. The desired value may be the maximum or the minimum value or be categorized into ordered categories. Examples of static problems are the maximum yield of a desired constituent during an isolation process, the minimum product loss during a manufacturing process, or the best sensory quality and acceptability of a food.

Dynamic problems are classified depending on the nature of the signal factor and the response variable (continuous or discrete). Examples of dynamic problems are fermentations in food processing in which the response (i.e., yield as product weight or concentration of a constituent, etc.), results by continuous monitoring of a process (viscosity increasing during curd formation in yogurt production, ethanol content increasing during wine fermentation).

C. Elements of Optimization Problems—Definitions

Optimization determines the values of independent variables that result in an optimal value of a dependent variable. This involves a process for finding the unique set of process conditions that produces the best results, usually after establishing a mathematical model of the product or process. The theory, methods, and techniques used to attain an optimum and to locate the optimum operating conditions are the subject of optimization. Following are definitions of the basic elements and terms that are common to all optimization problems (2, 4, 5). The representation of the relationship of the elements in an optimization problem and solution is in Fig. 2.

Performance function or objective function or response or criterion or criterion function or performance measure: This is a function of the design variables that quantifies the desired result. It is the measured variable that determines and reflects the performance of the system or process; it is the quantity to be optimized (maximized or minimized). It is often the profit, cost, product yield, energy consumption, and particularly for food systems the shelf life, consumer preference, quality characteristics, physical properties, etc.

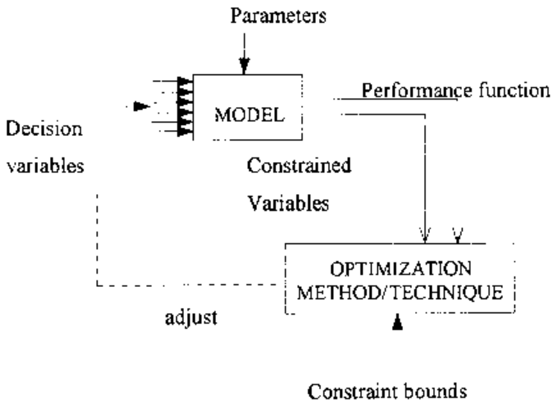

Figure 2 Elements of an optimization problem.

Decision (independent) variables or parameters or (control) factors: These are the parameters in the process that affect the value of the objective function and can be adjusted to improve performance. They are free and independent variables that must be specified in the process model. In food systems, these commonly include temperature, pressure, flow rates, pH, concentration, moisture content, concentration of ingredients, etc.

Constraints: These are the constraints on the allowed solutions that may have a problem to be optimized. The constraints, equality or inequality, limit the values of the dependent variables, the decision variables or even the performance functions of the process. Equality constraints are the fixed values that variables will have in the boundaries. Inequality constraints refer to upper or lower values of the variables that the system may approach at boundaries.

Mathematical model: The model is the mathematical representation of the process that determines the performance functions in terms of the decision variables or other independent variables subject to constraint. Modeling of a process is the application of engineering sciences and knowledge to describe mathematically (using mathematics, statistics, numerical analysis, computer software) a process and its performance. Simulation is the use of the model to assess different scenarios. The simulation of the process with a mathematical model facilitates the process optimization against to costly experiments predicting process results for any one set of decision variables. Furthermore, simulation helps to gain understanding, to evaluate alternatives, and to answer specific questions. Optimization is described as the simulation performed aiming to maximize (or minimize) a certain process objective; the search for the desired optimum is usually done using mathematical algorithms.

Optimization method or technique or procedure: This is the method of searching to find the optimum combination of decision variables possible within the boundary of the constraints. It can be as simple as selecting the combination among all possible combinations that produces the best results from the objective functions in the mathematical model. However, in complex problems where there are many decision variables with a wide range of values, a structured technique based on mathematical algorithms must be followed for solving of the problem. Computers and associated software make the computations involved in the selection (solution) feasible and cost-effective.

Feasible solutions: These are values of the design variables that satisfy all the constraints.

D. Problem Optimization Procedure

In a general case of optimization, the problem must first be formulated and then the system to be optimized must be defined. Following, a function (mathematical model) that describes the system must be constructed and then the system's optimum solution must be found. The simulation of the process by a mathematical model as well as the selection of the appropriate optimization method is fundamental to a successful process optimization. In all optimization problems, the above elements must be considered (6). A typical optimization problem procedure including the individual optimization steps and the relationships between the important optimization elements are presented in Fig. 3.

1. Optimization Problem Formulation

Formulation of problem optimization requires identifying the essential elements of a given system and organizing them into a mathematical form, namely: (a) the objective function (criterion) and (b) the process model and constraints (2). It means that the variables that affect the performance of the system and the variables that determine and reflect the system's behavior must be specified. The objective function represents profit in terms of the (key) variables of the process being analyzed and the process model and constraints describe the interrelationships of the (key) variables. A systematic approach for assembling the physical and empirical relations and data involved in an optimization problem and procedures are recommended.

The need for formulation of the problem has been illustrated by examples of relative optimization problems. Problem formulation and establishment of a satisfactory function that describes the behavior of the criterion as a function of the independent parameters is the most critical aspect in a problem optimization and usually the most difficult step of a successful optimization study; artistry, judgment, and experience is required during the problem formulation step of optimization.

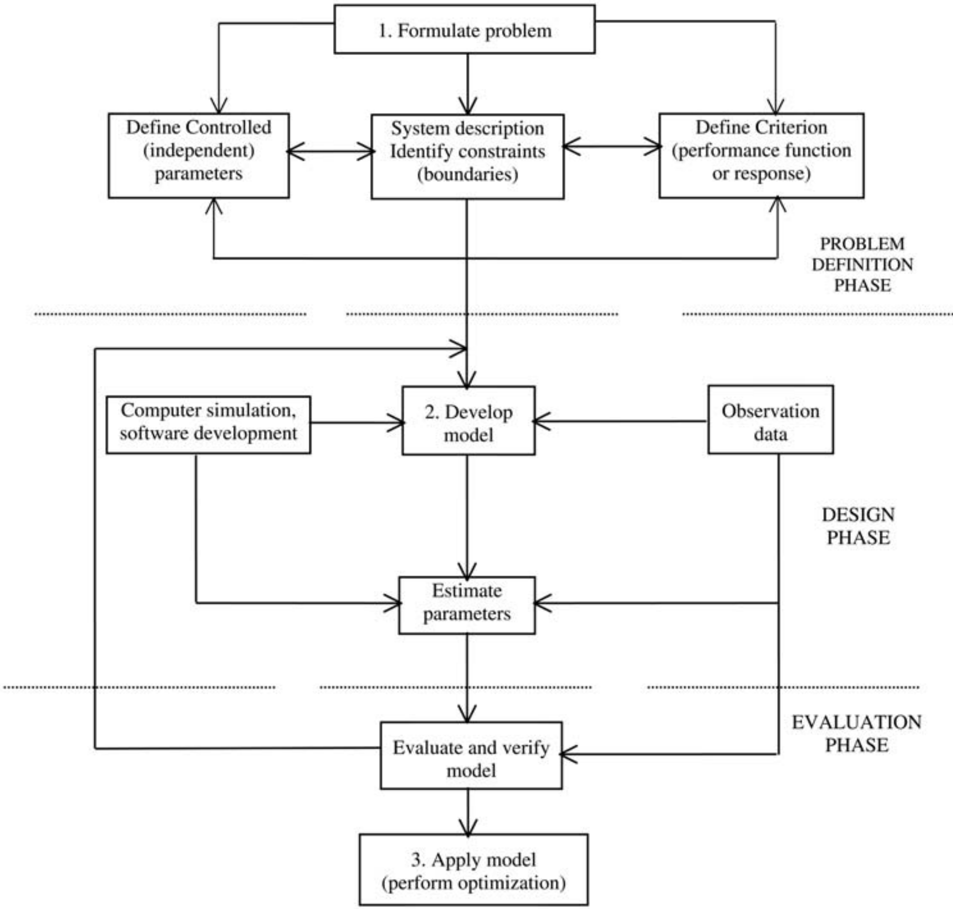

Figure 3 Problem optimization procedure.

For the formulation of problem optimization the following steps must be carried out:

1. Description of the system to be optimized. The system boundaries must be clearly defined so system parameters become independent of external parameters. All the subsystems that significantly affect the performance of the system should be included in the optimization problem. When dealing with complex systems, they are usually divided to subsystems that are optimized individually (suboptimization); similarly, during suboptimization the subsystem boundaries must be carefully selected.

2. Definition of a criterion (parameter). A single dependent parameter is defined, that serves as the overall evaluation criterion for the specific optimization problem. It will be maximized or minimized to satisfy the objectives and measures the degree the solution satisfies the desired objectives of the problem. Often, only one primary criterion is used as an optimization performance measure and all other criteria are treated as problem constraints or parameters. However, in complex problems, where the specification of the optimum solution is complicated by conflicting criteria, a single parameter must be established for optimization needs, taking into account the relative importance of all relevant criteria. In practice, if it is desirable to develop a design that is "best" with respect to many, usually competitive, criteria, advanced techniques for solving the optimization problem must be applied, i.e., simultaneously minimizing cost and environmental impact, while maximizing efficiency and reliability.

The selection of criteria on which the system design will be evaluated and optimized is a key element in formulating an optimization problem. Optimization criteria may be economical (total capital investment, total annual costs, annual net profit, return on investment), or technological (profitability evaluation criteria) (thermodynamic efficiency, production time, production rate, reliability, total weight, etc.), and environmental (e.g. emitted pollutants). An optimized design is characterized by a minimum or maximum value, as appropriate, for each selected criterion.

3. Definition of controlled or independent parameters. These are parameters that affect the performance of the process or system and can be adjusted, changed, and controlled. Their values determine the criterion parameter value and must lie within the boundaries of the defined problem. The most critical element in optimization problems is the selection of all the appropriate variables that contribute to the decision-making process of attaining the optimum. The variables must include all the important variables that affect the performance and cost effectiveness of the system, while not including details or variables of minor importance.

Functional and regional constraints: Functional constraints represent physical or functional interrelationships that exist among the independent parameters, while regional constraints limit the range over which the independent parameters can vary; they must be considered in addition to the parameters in optimization problems.

Other parameters: Formal optimization depends on a clear definition of the system to be optimized. It only works for the specific system described where all criteria and parameters are defined within the system and are isolated and independent from other parameters outside the boundaries of the system. Therefore, formal optimization theory should be used only to find optimum parameters in well-defined systems with unique, quantitative-dependent and -independent parameters, criterion function, and functional and regional constraints. So, the clearer the description of a given system, the more sure will be in obtaining the best solution. Furthermore, after the optimum set of parameters has been determined, other parameters, not included in the original problem, may be used and then compared with the others.

Suboptimization: It is usually applied to complex systems, where the optimization of the entire system may not be feasible, either due to the problem formulation or the inadequate optimization techniques. It can be also applied for economic and practical reasons. Then, the optimization of one subsystem as part of the whole problem is done, ignoring some variables that affect the objective function or other subsystems; it does not however ensure the optimization of the overall system.

2. Development of Mathematical Model—Design and Evaluation

The further procedures for formal optimization and solution techniques include the development of a model, model design, and application. That means the forming of the model, establishing and treating constraints, determining feasible solutions, and assigning of performance measures (6). In most cases of optimization, models are used instead of trial-and-error experiments and statistic techniques are applied.

Design includes general description and specification of the programming technique and algorithms, formulation of the mathematical description, and simulation of the model. In order to obtain a mathematical description of the process or system to be optimized, a mathematical model of the process or system is formed (7, 8).

A mathematical model is a description in terms of mathematical relations of the functions of a physical system; the way variables are interrelated and the independent variables affect the performance criterion are described by mathematical expressions. Models should closely represent the system and allow the determination of the performance functions in terms of the decision variables; consequently, development of a model requires a good understanding of the system.

The optimizer has to select the specific mathematical representation to be used in the model, as well as the assumptions and limitations of the model. All the important aspects of the problem should be included, so that they will be taken into account in the solution (specific values of the variables, assigned variables that are functions of time, other independent variables, satisfaction of constraints or certain goals, etc.). Care must be taken not to omit any significant factor to save time. The degree of accuracy needed in the model must be determined. A successfully developed model helps to solve of the optimization problem. Process design simulations and flow-sheeting software are also very useful during modeling. Model building is completed by evaluation and application; it is an iterative process as improved models can be produced by feedback of information.

The mathematical model for an optimization problem consists of:

1. Objective function to be maximized or minimized

   $f(x)$ objective function (a)

2. Equality and inequality constraints

   $h(x) = 0$ equality constraints (b)

   $g(x) \geq 0$ inequality constraints (c)

where x is a vector of n variables $(x_1, x_2, \ldots, x_n)$, $h(x)$ is a vector of m_1 equations, and $g(x)$ is a vector of m_2 inequalities. The total number of constraints is $m = (m_1 + m_2)$.

1. The objective function expresses the optimization criterion (C) as a function of the dependent and independent variables $(x_1, x_2, \ldots, x_n)$ and may be represented by:

$$C = f(x_1, \ldots, x_n) \qquad \text{optimization criterion function} \qquad \text{(d)}$$

The equality and inequality constraints are provided by appropriate models as well as by appropriate boundary conditions. These models usually may be a cost function, a benefit or profit function, or functions associated with material and energy balance with engineering design. The models also contain equations and inequalities that specify the allowable operating ranges, the maximum or minimum performance requirements, and the bounds on the availability of resources.

System models may be linear or nonlinear (set of algebraic, differential, or partial differential equations), static (focused on steady-state operation), or dynamic (focused on transient state), deterministic (not allowing variations), or stochastic (or probabilistic with time-varying parameters). Mathematical models exist for some food processes; for the rest they must be developed based on relevant engineering and scientific knowledge. Their complexity varies depending on the application, so in some food systems model development may be difficult or impossible. Then, an approximating function is developed as closely as possible to the system by performing an appropriate experimental design with limited number of experiments and by model-fitting techniques.

2. The constraints, which in most optimization problems may limit the values of dependent or independent variables and consequently the region of allowable solutions, must be identified. Constraints may be imposed by the particular characteristic of the system or represent external restrictions (equipment, legal, etc.). The system model must account for all the imposed constraints.

Constraints restrict the values of the system variables. Constraints often are classified as being either equality or inequality constraints. The types of constraints involved in any given problem are determined by the physical nature of the problem and by the level of complexity used in forming the mathematical model.

Constraints may be rigid, referred to as physical variables (restricted to non-negative), government regulations, or customer requirements, etc., or may be soft-negotiable to some degree (soft constraints). The former are viewed as absolute goals, while the latter as goals associated with target values.

Functional constraints: These are physical principles of operation, which govern the relationship among the various independent parameters ($x_1, x_2, \ldots, x_n$) of the problem and are represented by equations:

$$fc_i = f_i(x_1, x_2, \ldots, x_n) \tag{e}$$

Regional Constraints: These are practical limits on the range in which each parameter (x_i) or function of the parameters can be varied and are expressed as inequalities:

$$l_1 \leq r_i(x_1, x_2, \ldots, x_n) \leq l_2 \tag{f}$$

In an optimization problem, functional constraints can be used to eliminate the number of independent parameters. Normally, the number of functional constraints must be less than the number of independent parameters, while there can be any number of regional constraints.

Feasible solutions: After the constraints are established, the existence of feasible solutions for the given problem (points or region) that simultaneously satisfy all of the constraints must be examined, whereas the soft constraints may be relaxed in order to minimize the deviations from goals.

Evaluation of the model: This is carried out according to the evaluation criteria established in the problem definition and sensitivity testing of the model inputs and parameters. Use actual data, which may entail statistical analysis of the fitted parameters, in the model when possible.

Fitting functions to empirical data: A model relates the output, i.e., the dependent variable(s) to the independent variable(s). Each equation in the model usually includes one or more coefficients that are presumed constant. The term *parameter* as used here will mean coefficient and possibly input or initial condition. With the help of experimental data, the form of the model can be determined, and subsequently (or simultaneously) the value of some or all of the parameters in the model estimated.

Model validation: This consists of validation of model assumptions and model behavior by comparison with historical input–output, literature, and performance data and simulation. In general, data used in formulating a model should not be used to validate it. No single validation procedure is appropriate for all models. The model should predict the desired features of the process performance with suitable accuracy.

3. Performing of Optimization—Attaining the Optimum

During the final step of the problem optimization process—attaining the optimum—the optimization must be performed by the appropriate selected method (5). Optimization methods have as scope to adjust, re-adjust, and locate the values of the decision variables that optimize (maximize or minimize) the performance function, while insuring that all variables (dependent or independent) satisfy the constraints of the system.

The already developed model of the system usually dictates the approach of optimal solution. Such approaches are: unconstrained optimization, constrained optimization with a single performance measure or multiple performance measures, and optimization of systems that evolve over time (dynamic optimization).

Assigning of performance measures: The performance measures that are to be optimized must be assigned (6). The selection of meaningful performance measures is critical for the optimization results. Usually, one of the performance measures is assigned as a target and the remaining are converted into soft constraints. Performance measures are incorporated into the optimization process either by contacting actual experiments or using numerical searching techniques.

Solution of optimization problems: The reliability of the solutions of optimization problems depends on well-defining the problems. In complex problem optimization, initial considerations may be primarily based on the optimizer's judgments of the relevant parameters until a clearer configuration of the problem parts can be defined, together with the relevant criteria, parameters, and constraints. Procedures for defining competing systems or alternate strategies and formulating the problem in order to apply formal optimization techniques are also common to operations research, systems analysis, and systems design.

The general formal optimization problem is formulated in terms of the three previously referred equations: the criterion function, and the functional and regional constraints. The techniques used for solving the optimization problem depend on the complexity of the optimization equations. Detailed treatment of the various techniques for solving of equations represent the literature about optimization.

Consequently, the formulation and solution of an optimization problem involves the establishment of an evaluation criterion based on the problem objectives, followed by the determination of the optimum values of the controllable or independent parameters that will best satisfy the evaluation criterion. It is accomplished either by performance of measures or analytically. In most optimization problems where there are conflicting criteria a compromise must be done weighting their relative value.

III. OPTIMIZATION METHODS

A mathematical theory of optimization has been developed and has found application in a variety of engineering situations (1, 2, 5, 9, 10). The development of the digital computer allowing rapid numerical calculations has made the utilization of optimization procedures practical in many design situations.

Mathematical programming techniques are useful in finding the minimum of a function of several variables under a prescribed set of constraints. Stochastic process techniques can be used to analyze problems described by a set of random variables having known probability distributions. Statistical methods enable one to analyze the experimental data and build empirical models to obtain the most accurate representation of the physical situation.

An optimization or a mathematical programming problem can be stated as follows:

$$\text{find } X = \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{Bmatrix} \text{ which minimizes or maximizes } f(X)$$

in unconstrained optimization problems or

$$\text{find } X = \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{Bmatrix} \text{ which minimizes or maximizes } f(X) \text{ under the constraints:}$$

$$h_j(X) \le 0, j = 1, 2, \ldots\ldots, m$$
$$g_j(X) = 0, j = 1, 2, \ldots\ldots, p$$

in constrained optimization problems, where X is an n-dimensional vector called the design vector and f(X) is termed the objective function; in the case of constrained problems $h_j(X)$ and $g_j(X)$ are known as inequality and equality constraints, respectively. The minimizing/maximizing point or minimizer/maximizer is denoted by x*.

A. Basic Theoretical Background (1, 2, 9, 10)

In any engineering system the design vector, defined during the design process by a set of variables, represents the selected design variables as X:

$$X = \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{Bmatrix} \text{ where } x_i \text{ are the design variables } i = 1, 2, \ldots, n.$$

A vector is also represented by x and usually refers to a column vector. A matrix is referred as X and its elements as X_{ij} or x_{ij}. A column vector of n variables is also represented in n-dimensional space R^n by: $x = [x_1, x_2, \ldots, x_n]^T$, where the superscript T signifies the transpose of a row vector to form the column vector x.

In the n-dimensional space (R^n), each coordinate axis represents a design space (or design variable space). A point x in n-dimensional space is the vector $(x_1, x_2, \ldots, x_n)^T$, where x_i is the component in the i-coordinate direction. For a given function f(x) of n variables, points at which f(x) assumes local maximum and local minimum values are of interest. Each point in the n-dimensional design space, called design point, represents either a possible or an impossible solution to the design problem. Optimization methods by iterative processes generate a sequence of points $x^{(k)}$ or $\{x^{(k)}\}$(where k is the iteration number) intending to find x*, the solution of the problem.

In general, it is assumed that the problem functions are smooth, continuous and continuously differentiable (C^1). Therefore for a function f(x) at any point x, there is a vector of first partial derivatives, or gradient vector.

$$\nabla f(x) = \begin{Bmatrix} \partial f/\partial x_1 \\ \partial f/\partial x_2 \\ \vdots \\ \partial f/\partial x_n \end{Bmatrix}$$

where ∇ denotes the gradient operator $(\partial f/\partial x_1, \partial f/\partial x_2, \ldots\ldots, \partial f/\partial x_n)^T$. If f(x) is twice continuously differentiable (C^2), then there is a matrix of second partial derivatives $\nabla^2 f(x)$ with elements $\partial^2 f/(\partial x_i\, \partial x_j)$ that is called Hessian matrix and denoted by H(x). This matrix is square and symmetric. Since any column is $\nabla(\partial f/\partial x_j)$, the matrix can be written as $\nabla(\nabla f^T)$.

Special cases of many variable functions include the general linear function, which can be written as:

$$l(x) = \sum_{i=1}^{n} a_i x_i + b_i = a^T x + b$$

where a and b are constants. The general quadratic function, can be written as:

$$q(x) = \tfrac{1}{2} x^T G x + b^T x + c$$

where G, b, and c are constant and G is symmetric.

The basis for all optimization methods is the classic theory of maxima and minima. Mathematically, the theory concerned with finding the minimum or maximum (extreme points) of an unconstrained function of n variables $f(x_1, x_2, \ldots, x_n)$ that can be interpreted geometrically as finding the point in an n-dimension space at which the function has an extremum. An optimal point x* is completely specified by satisfying the necessary and sufficient conditions for optimality.

Following the desirable features of functions, as well as the necessary sufficient conditions to guarantee the defined extremum (minimum or maximum), are presented. The knowledge of the basic properties of objective functions and constraints is considered necessary.

It is preferable and more convenient to work with continuous functions of one or more variables as well as with functions having continuous derivatives. Then the extreme points may lie at the stationary points and consequently a necessary condition for a minimum or maximum is:

$f'(x) = 0$ or $\nabla f(x) = 0$ (except in case of saddle points).

Hence, in order to locate the points where the partial derivatives are zero, the solving of n-algebraic equations should be done: $\partial f/\partial x_j (x_1, x_2, \ldots, x_n) = 0$ ($j = 1, \ldots, n$). The equations can be solved directly or in some cases an approximate solution can be obtained by minimizing the sum of squares of the residuals (least squares method).

It is also better to work with a unimodal function that has a single extremum (minimum or maximum); that is, a stationary point. Multimodal function has two or more extrema (maximum or minimum); these are multiple stationary points. The global extremum is the biggest or smallest among a set of extrema; local extrema may be significant in practical optimization problems involving nonlinear functions. Sufficient conditions for a unique (isolated) or extremum to exist are:

$f''(x) = \nabla^2 f(x) = H(x) > 0$ for unique (global) minimum
$f''(x) = \nabla^2 f(x) = H(x) < 0$ for unique (global) maximum
$f''(x) = \nabla^2 f(x) = H(x) = 0$ neither maximum nor minimum (inflection point).

The determination of convexity or concavity is helpful to establish if a local optimal solution is also a global optimal solution. A convex region is useful in optimization involving constraints. Equality constraints limit the feasible set of points on hyper-surfaces, curves, or even a single point, while inequality constraints specify a feasible region comprised of the set of points that are feasible.

To simplify the above, the case of a function of one variable x is assumed. A point x^* is called local minimum if $f(x^*) \le f(x + h)$ for all sufficiently small positive and negative values of h. Similarly, a point x^* is called a local maximum if $f(x^*) \ge f(x + h)$ for all values of h close to zero. A point x^* will be a global minimum at x^* if $f(x^*) \le f(x)$ or a global maximum of $f(x)$ if $f(x^*) \ge f(x)$ respectively for all x, and not just for all x close to x^*, in the domain over which $f(x)$ is defined.

Examples of local and global optimum points are presented in Fig. 4. Local minimum or maximum can be located at the boundaries or at points at

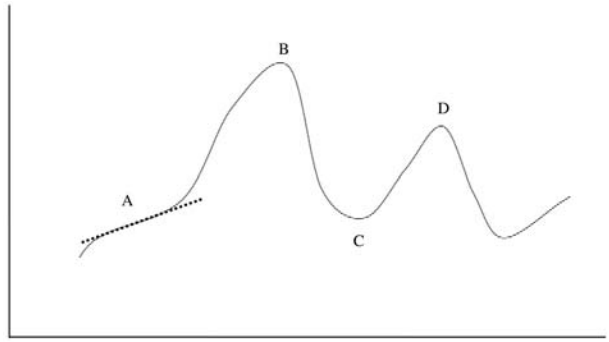

Figure 4 Types of stationary points of a function. A, inflection point (scalar equivalent to a saddle point); B, global maximum; C, local minimum; D, local maximum.

which the first derivative (f′) is zero or discontinuous (stationary points). One of the local minimum/maximum can be a global minimum/maximum. Points whose first derivative is zero, may be neither a maximum nor a minimum, but a mini-max, or better known as a saddle point and movement away form it will result in an increase or decrease on f(x) depending on the direction of the movement. Difficulties are caused when f(x) is a non-smooth function as its minima do not satisfy the same conditions as smooth minima.

B. Basic Optimization Methods

Many methods have been developed for the efficient solution of optimization problems; there is no general mathematical method for conducting the search for the optimal value.

The optimization methods can be categorized according to: (a) the nature of the objective function; (b) the constraints; and (c) the decision variables involved.

The *objective function* may:

1. Contain only a single decision variable (single or one-dimensional optimization) or many decision variables (multidimensional optimization)
2. Be continuous or contain discontinuities, and
3. Be linear or nonlinear (linear programming—LP or nonlinear programming—NLP)
4. Be one or more than one (single or multi-objective programming)

Constraints may or may not exist in a problem and constrained or unconstrained optimization are the two main categories. The constraints may be expressed as linear or nonlinear equations or inequalities.

The *decision variables* may be continuous, integers, or a combination. Depending on the nature of the design variables static or dynamic optimization methods may exist. Also, based on the deterministic nature of the variables, deterministic, or stochastic programming is classified.

Graphical methods involve a procedure of finding a maximum or minimum point of the objective function by the graphical plotting of the objective function values. These methods are elementary, have reduced accuracy and are usually applied in the case of one or two-variable functions.

Methods may be *indirect or direct*. Indirect methods determine extremum (a) by using derivatives and values of the objective function. A necessary condition for an extremum point of a differentiable objective function is that the point is a stationary point. Direct methods search for an extremum by directly comparing function values at a sequence of trial points without involving derivatives. These methods generally can more easily treat problems involving objective functions with discontinuities, points of inflection, and boundary points, while computers have enabled their application.

Numerical methods are search techniques that have been developed to determine maxima and minima of functions. The objective function is computed at a starting set of the independent variables. A second set is then selected and the comparison of the new value of the objective function with the initial one indicates if the objective function is improving toward an optimum. Searches are simultaneous, when all sets of evaluation values are preselected, or are sequential when new sets of data are selected based on information from the previous sets of data. In applying numerical optimization methods, their efficiency should be taken into account before selecting the appropriate optimization method.

When the objective function is continuous and continuously differentiable and not near the region limits, the optimization may be done *analytically*. This implies solving a set of differential equations of the first derivatives of the objective function with respect to each independent variable and following the usual mathematical procedures for maxima and minima. Additional mathematical procedures include the use of Lagrange multipliers and variational calculus.

Given that a function and its derivatives are continuous, a method that exhibit quadratic convergence may be best; such methods can locate the exact maximum/minimum of a quadratic function (assuming it has a well-defined optimum) in a finite number of calculations.

Gradient-based methods are search techniques that use derivatives; the gradient vector $\nabla f(x)$ is central to these methods. At each point the gradient vector is perpendicular to the contour of the function and points in the direction of the greatest incremental increase in f(x). The gradient search works as follows: (a) evaluate a search direction $r = \nabla f(x)$ at the current best $x = x^0$; (b) let $x = x^0 + \nu r$, where ν is a real scalar; (c) search for a maximum of f with respect to values of $\nu \geq 0$; and (d) reassign the current best x and return to step (a). This method is simple, however is inefficient when the contours are elongated or irregular in any way.

Following, the usual cases of a single-variable function or a multivariable function with no constraints, and a multivariable function with equality and inequality constraints are presented. Also, some commonly used techniques applicable to these types of optimization problems are briefly discussed (1, 2, 5, 9–12).

1. Unconstrained Optimization

Unconstrained optimization methods are applicable when searching for a minimum or maximum of a function that is not subject to any constraints. Unconstrained optimization may be single or one-dimensional or multi-dimensional optimization.

Single or One-Dimensional Unconstrained Optimization. This is the most elementary type of optimization problem; the function f(x) has only one independent variable. The techniques applicable to this type of problem are important because some techniques applicable to multivariable functions involve repeated use of a single-variable search.

To develop the necessary and sufficient conditions for a minimum or maximum of a function f(x), a Taylor series expansion (with n terms) about the presumed extremum x* can be performed.

$$f(x^* + h) = f(x^*) + hf'(x^*) + \frac{h^2}{2!} f''(x^*) + \dots + \frac{h^{n-1}}{(n-1)!} f^{(n-1)}(x^*) + \frac{h^n}{n!} f^{(n)}(x^* + \theta h) \qquad \text{for } 0 < \theta < 1 \tag{1}$$

If $f'(x^*) = f''(x^*) = \dots = f^{(n-1)}(x^*) = 0$, but $f^{(n)}(x^*) \neq 0$
then

$$f(x^* + h) - f(x^*) = \frac{h^n}{n!} f^{(n)}(x^* + \theta h) \tag{2}$$

$f(x^*)$ is a minimum if $f^{(n)}(x^*) > 0$ and n is even, $f(x^*)$ is a maximum if $f^{(n)}(x^*) < 0$ and n is even, and neither a minimum nor a maximum (inflection point) if n is odd.

For example when $n = 2$, given that $f'(x^*) = 0$ at the stationary point, the higher order terms are negligible compared to the second-order terms and hence equation becomes:

$$f(x^* + h) = f(x^*) + \frac{h^2}{2!} f''(x^*) \tag{3}$$

Then, the nature of $f(x^*)$ depends on the value of $f''(x^*)$ as already referred. That is at x* exists a minimum if $f''(x^*) > 0$, a maximum if $f''(x^*) < 0$ or an inflection point if $f''(x^*)$ is indefinite.

Multidimensional Unconstrained Optimization. The theory for the minimum or maximum applied in one-dimensional optimization is generalized and extended in the case of a function of n independent variables. Therefore, for the necessary and sufficient conditions for minimum or maximum of an unconstrained function of several variables, the Taylor's series expansion of a multivariable function about a point X* is:

$$f(X) = f(X^*) + d\,f\,(X^*) + \frac{1}{2!}\,d^2 f\,(X^*) + \ldots + \frac{1}{N!}\,d^N f(X^*) + R_N\,(X^*, h) \qquad (4)$$

where the last term, called the remainder, is given by:

$$R_N\,(X^*, h) = \frac{1}{(N+1)!}\,d^{N+1} f(X^* + \theta\,h) \qquad (5)$$

where $0 < \theta < 1$ and $h = X - X^*$.

It must he noted that the *r*th differential of f(x) at X* (partial derivative of *r* order) is the polynomial:

$$d^r f(X^*) = \underbrace{\sum_{i=1}^{n} \sum_{j=1}^{n} \cdots \sum_{k=1}^{n}}_{\text{r summations}} h_i h_j \ldots h_k \frac{\partial^r f(X^*)}{\partial x_i \partial x_j \cdots \partial x_k} \qquad (6)$$

The necessary condition for f(X) having an extreme point (maximum or minimum) at $X = X^*$ is the first partial derivatives of f(X) to exist at X* and to be 0.

$$\frac{\partial f}{\partial x_1}(X^*) = \frac{\partial f}{\partial x_2}(X^*) = \ldots = \frac{\partial f}{\partial x_n}(X^*) = 0 \qquad (7)$$

A sufficient condition for a stationary point X* to be an extreme point depends on the nature of the matrix of second partial derivatives (Hessian matrix) of f(X*). This results to the quantity Q (given that $\frac{\partial f}{\partial x_i}(X^*) = 0$ for $i = 1, \ldots, n$ and second partial derivatives of $\frac{\partial^2 f}{\partial x_i x_j}(X^*)$ are continuous in the vicinity of X*):

$$Q = \sum_{i=1}^{n} \sum_{j=1}^{n} h_i h_j \frac{\partial^2 f(X^*)}{\partial x_i \partial x_j} = h^T\,J\,h\,\big|_{x=x^*} \qquad (8)$$

where $J\Big|_{x=x^*} = \left[\frac{\partial^2 f}{(\partial x_i\,\partial x_j)}\Big|_{x=x^*}\right]$ is the Hessian matrix of f(X). Consequently, if

$J|_{x=x^*} > 0$ then X* is a relative minimum point, and if $J|_{x=x^*} < 0$ then X* is a relative maximum point. In case that the Hessian matrix is semidefinite (but not definite), the stationary points should be investigated for sufficiency in actual practice.

However, in the general case where the partial derivatives of f of all orders up to the order $k \geq 2$ are continuous in the vicinity of a stationary point X*, and

$$d^{k-2}|_{x=x^*} = 0$$

$$d^k|_{x=x^*} \neq 0 \text{ (the first nonvanishing higher-order differential of f at X*)}$$

then, if k is even, when $d^k|_{x=x^*} > 0$, X* is a relative minimum point, when $d^k|_{x=x^*} < 0$, X* is a relative maximum point, and when $d^k|_{x=x^*}$ is semidefinite (but not definite), no general conclusion can be drawn (X* is not an extreme point, if k is odd).

In the case of a function of two variables f(x,y), the Hessian matrix may be neither positive nor negative definite at a point (x*,y*) at which $\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} = 0$. That point is a saddle point.

Unconstrained nonlinear multivariable optimization. The unconstrained nonlinear programming methods used for multivariable optimization are iterative procedures in which the following two steps are repeated: (a) starting from a given point choose a search direction and (b) minimize or maximize in that direction to find a new point. These methods mainly differ in how they generate the search directions.

Direct/indirect methods. Direct methods for single variable functions include the region elimination methods, the two-point equal interval search, the bisecting method (or dichotomous search), the Fibonacci method, and the golden section method; the last two methods are considered the most efficient. The point estimation methods, or polynomial approximation methods usually involve a quadratic or cubic approximation of the objective function and for this Powell's method is considered the most efficient.

For multivariable functions, direct methods include the random search, the grid search, the univariate search, the sequential Simplex method, the Hooke-Jeeves pattern search method, and Powell's conjugate direction method. These methods are relatively simple to understand and execute. However, they are not as efficient and robust as many of the indirect methods.

The indirect methods include the steepest descent/ascent gradient method (or Cauchy's method), the conjugate gradient methods, Newton's method, Marquardt's method, the Secant methods, and the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method.

2. Constrained Optimization

Constrained optimization methods are applicable to locate stationary points of a function, but the solutions are subject to equality or inequality constraints.

Optimization of the function must be carried out over a restricted domain of the independent variables.

Optimization of Systems with Equality Constraints. Constrained optimization of a continuous function $f(x_1, x_2, \ldots, x_n)$ of n independent variables subjected to m equality constraints $g_i(x_1, x_2, \ldots, x_n)$ $(i = 1, 2, \ldots, m)$ will be considered. The problem is defined when $m \leq n$.

Three methods are mainly used for the solution of such problems: direct substitution, constrained variation, and Lagrange multipliers.

Direct substitution methods involve the substitution of the m constraint equations directly into the objective function. The resulted objective function is not subject to any constraint and hence its optimum can be found by applying the unconstrained optimization techniques. This method is suitable for solving simpler problems, but cannot be applied to many practical problems due to nonlinearity of the constraints equations.

Constrained variation methods in the general case of n variables with m constraints scope in finding an expression for the first-order differential of f (df) at all points where the constraints are satisfied. Each constraint equation is expressed as a linear equation of the variations dx_i, $i = 1, 2, \ldots, n$ (m equations of n variations). Each one of m variations as well as df are expressed by the remaining n-m variations. The optimum points are obtained when $df = 0$.

$$\begin{aligned}
df &= \frac{\partial f}{\partial x_1} dx_1 + \ldots\ldots + \frac{\partial f}{\partial x_n} dx_n = 0 \\
dg_1 &= \frac{\partial g_1}{\partial x_1} dx_1 + \ldots\ldots + \frac{\partial g_1}{\partial x_n} dx_n = 0 \\
&\qquad \ldots\ldots\ldots\ldots \\
dg_m &= \frac{\partial g_m}{\partial x_1} dx_1 + \ldots\ldots + \frac{\partial g_m}{\partial x_n} dx_n = 0
\end{aligned} \tag{9}$$

Hence, the necessary conditions for the extremum of f(X) are given by the n-m equations (Jacobian determinants):

$$J\left(\frac{f, g_1, g_2, \ldots, g_m}{x_k, x_1, x_2, \ldots, x_m}\right) = \begin{vmatrix}
\frac{\partial f}{\partial x_k} & \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \cdots & \frac{\partial f}{\partial x_m} \\
\frac{\partial g_1}{\partial x_k} & \frac{\partial g_1}{\partial x_1} & \frac{\partial g_1}{\partial x_2} & \cdots & \frac{\partial g_1}{\partial x_m} \\
\frac{\partial g_2}{\partial x_k} & \frac{\partial g_2}{\partial x_1} & \frac{\partial g_2}{\partial x_2} & \cdots & \frac{\partial g_2}{\partial x_m} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{\partial g_m}{\partial x_k} & \frac{\partial g_m}{\partial x_1} & \frac{\partial g_m}{\partial x_2} & \cdots & \frac{\partial g_m}{\partial x_m}
\end{vmatrix} = 0 \tag{10}$$

where $k = m + 1, m + 2, \ldots\ldots, n$.

Similarly, in the case of two independent variables x_1, x_2 where the function $f(x_1,x_2)$ is subject to the constraint $g(x_1,x_2)$, a necessary condition for f to have an extreme point at (x_1^*,x_2^*) is:

$$df = \frac{\partial f}{\partial x_1}\, dx_1 + \frac{\partial f}{\partial x_2}\, dx_2 = 0 \tag{11}$$

$$dg = \frac{\partial g}{\partial x_1}\, dx_1 + \frac{\partial g}{\partial x_2}\, dx_2 = 0 \tag{12}$$

or by combining the equations:

$$\left(\frac{\partial f}{\partial x_1} \frac{\partial g}{\partial x_2} - \frac{\partial f}{\partial x_2} \frac{\partial g}{\partial x_1} \right) \bigg|_{(x1^*,\ x2^*)} = 0 \tag{13}$$

It is noted that the variations dx_1, dx_2 about the point (x_1^*,x_2^*) are called admissible variations.

A sufficient condition for X* to be a constrained relative extremum is resulted by the Taylor series expansion of f, in terms of n-m variables (x_{m+1}, $x_{m+2}, \ldots, x_n$) about the extremum point X*:

$$f(X^* + dX) \approx f(X^*) + \sum_{i=m+1}^{n} \left(\frac{\partial f}{\partial x_i} \right)_g dx_i + \frac{1}{2!} \sum_{i=m+1}^{n} \sum_{j=m+1}^{n} \left(\frac{\partial^2 f}{\partial x_i \partial x_j} \right)_g dx_i dx_j \tag{14}$$

where $\left(\frac{\partial f}{\partial x_i} \right)_g$ and $\left(\frac{\partial^2 f}{\partial x_i \partial x_j} \right)_g$ are the first and second partial derivatives of f with respect to x_i and x_i x_j (holding all the n-m variables constant) respectively, when $x_1, x_2, \ldots, x_m$ are allowed to change so that the constraints $g_j\ (X^* + dX) = 0$, $j = 1, 2, \ldots, m$, are satisfied.

The quadratic form Q defined by:

$$Q = \sum_{i=m+1}^{n} \sum_{j=m+1}^{n} \left(\frac{\partial^2 f}{\partial x_i \partial x_j} \right)_g dx_i dx_j \tag{15}$$

or the matrix:

$$\begin{bmatrix} \left(\frac{\partial^2 f}{\partial x_{m+1}^2} \right)_g & \left(\frac{\partial^2 f}{\partial x_{m+1} \partial x_{m+2}} \right)_g & \cdots & \left(\frac{\partial^2 f}{\partial x_{m+1} \partial x_n} \right)_g \\ \vdots & \vdots & \ddots & \vdots \\ \left(\frac{\partial^2 f}{\partial x_n \partial x_{m+1}} \right)_g & \left(\frac{\partial^2 f}{\partial x_n \partial x_{m+2}} \right)_g & \cdots & \left(\frac{\partial^2 f}{\partial x_n^2} \right)_g \end{bmatrix} \tag{16}$$

depending on their positive or negative value for all nonvanishing variations

dx_i are determinant for the optimum point X*. This method involves difficult computations as the constraints are more than two.

Lagrange Multipliers method is the most commonly used method in constrained optimization problems with equality constraints. The Lagrange function L, for a problem of n variables and m equality constraints is defined for each constraint g_j (X) as:

$$L(x_1, x_2, \ldots, x_n, \lambda_1, \lambda_2, \ldots, \lambda_m) = f(X) + \lambda_1 g_1(X) + \lambda_2 g_2(X) + \ldots\ldots + \lambda_m g_m(X) \tag{17}$$

where the quantities λ_j are called Lagrange multipliers.

The necessary conditions for the extremum of L are produced by the solution of a system of n+m equations in terms of the unknowns, x_i and λ_j, and are given by:

$$\frac{\partial L}{\partial x_i} = \frac{\partial f}{\partial x_i} + \sum_{j=1}^{m} \lambda_j \frac{\partial g_j}{\partial x_i} = 0, \; i = 1, 2, \ldots, n \tag{18}$$

$$\frac{\partial L}{\partial \lambda_j} = g_j(X) = 0, \; j = 1, 2, \ldots, m \tag{19}$$

From the solution, the relative constrained extremum X* and the λ* result. It must be noted that the vector λ* of Lagrange multipliers is a sensitivity factor that indicates how tightly the constraint is binding at the optimum point.

A sufficient condition for f(X) to have a relative extremum at X* is determined by the sign of the quadratic form Q:

$$Q = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial^2 L}{\partial x_i \partial x_j} (X^*, \lambda^*) \; dx_i dx_j \tag{20}$$

or by the sign of the roots of the polynomial z_i:

$$z_i = \begin{vmatrix} L_{11-z} & L_{12} & \cdots & L_{1n} & g_{11} & g_{21} & \cdots & g_{m1} \\ L_{21-z} & L_{22} & \cdots & L_{2n} & g_{21} & g_{22} & \cdots & g_{m2} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ L_{n1-z} & L_{n2} & \cdots & L_{nn-z} & g_{1n} & g_{2n} & \cdots & g_{mn} \\ g_{11} & g_{12} & \cdots & g_{1n} & 0 & 0 & \cdots & 0 \\ g_{21} & g_{22} & \cdots & g_{2n} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ g_{m1} & g_{m2} & \cdots & g_{mn} & 0 & 0 & 0 & 0 \end{vmatrix} = 0 \tag{21}$$

$$\text{where } L_{ij} = \frac{\partial^2 L}{\partial x_i \; x_j} (X^*, \lambda^*), \; g_{ij} = \frac{\partial g_i}{\partial x_j} (X^*) \tag{22}$$

So, if Q or each root of z_i is positive or negative for all values of dX, X* will be a constrained minimum or maximum respectively. It must be noted that the point X^* is not an extreme point if all of the roots of z_i have not the same sign.

The solution of a simple two-dimensional problem by Lagrange multipliers method is:

$$L(x_1, x_2, \lambda) = f(x_1, x_2) + \lambda\, g(x_1, x_2) \tag{23}$$

Then, the necessary conditions for the extremum X^* (x_1, x_2) are given by:

$$\frac{\partial L}{\partial x_1}(x_1, x_2) = \frac{\partial f}{\partial x_1}(x_1, x_2) + \lambda \frac{\partial g}{\partial x_1}(x_1, x_2) = 0 \tag{24}$$

$$\frac{\partial L}{\partial x_2}(x_1, x_2) = \frac{\partial f}{\partial x_2}(x_1, x_2) + \lambda \frac{\partial g}{\partial x_2}(x_1, x_2) = 0 \tag{25}$$

$$\frac{\partial L}{\partial \lambda}(x_1, x_2, \lambda) = g\,(x_1, x_2) = 0 \tag{26}$$

Optimization of Systems with Inequality Constraints. Constrained optimization subject to inequality constraints is treated as in the case of equality constrained problems after transformation of inequality constraints to equality ones by introducing the slack variables and solving the so formed constrained equations to define the feasible region and find the optimum solution. A usual problem of this category is the linear multivariable optimization with inequality constraints.

For the general case of a function f (X) of n independent variables subject to m constraints $g_j(X) \le 0$ $(j = 1, 2, \ldots, m)$, the constraints are transformed to equality ones as:

$$g_j(X) + y_j^2 = 0 \quad (j = 1, 2, \ldots, m) \tag{27}$$

where y_i are non-negative slack variables.

Hence, the problem becomes the finding of the extremum of f(X) subject to:

$$G_j(X, Y) = g_j(X) + y_j^2 = 0 \quad (j = 1, 2, \ldots, m) \tag{28}$$

where Y is the vector of slack variables and can be solved by using the previously referred Lagrange multipliers method as:

$$L(X, Y, \lambda) = f(X) + \sum_{j=1}^{m} \lambda_j G_j(X,Y) \tag{29}$$

where λ is the Lagrange multipliers vector.

Then, applying the necessary conditions for the stationary points, the following $(n + 2m)$ equations of $(n + 2m)$ unknowns result:

$$\frac{\partial L}{\partial x_i}(X, Y, \lambda) = \frac{\partial f}{\partial x_i}(X) + \sum_{j=1}^{m} \lambda_j \frac{\partial g_j}{\partial x_i}(X) = 0, \ i = 1, 2, \ldots, n \tag{30}$$

$$\frac{\partial L}{\partial \lambda_j}(X, Y, \lambda) = G_j(X, Y) = g_j(X) + y_j^2 = 0, \ j = 1, 2, \ldots, m \tag{31}$$

$$\frac{\partial L}{\partial y_j}(X, Y, \lambda) = 2 \lambda_j y_j^2 = 0, \ j = 1, 2, \ldots, m \tag{32}$$

3. Optimization of Dynamic Systems

A dynamic system is characterized by time- or space-dependent behavior and variety by time or distance. The problems are called sequential decision problems or multistage decision problems as the decisions are to be made sequentially or at a number of stages respectively. Many dynamic systems are encountered in chemical engineering and food engineering (fermentations or thermal processes of foods).

For the optimization of multistage decision problems, dynamic programming techniques are used. Dynamic programming methods decompose an optimization problem into a sequence of subproblems that can be solved serially. Each of the subproblems may contain one or few decision variables.

A serial multistage decision process of n stages in decreasing order is represented schematically in Fig. 5. Each single-stage i decision process can be characterized by an input (input state parameter) (S_{i+1}) which is the output of i + 1 stage, a decision variable (X_i), an output (output state parameter) (S_i) and a return or objective function (R_i). The output is obtained as a result of making the decision, while the return depends on the effectiveness of the decision made and the output that results from the decision. The state transformation functions

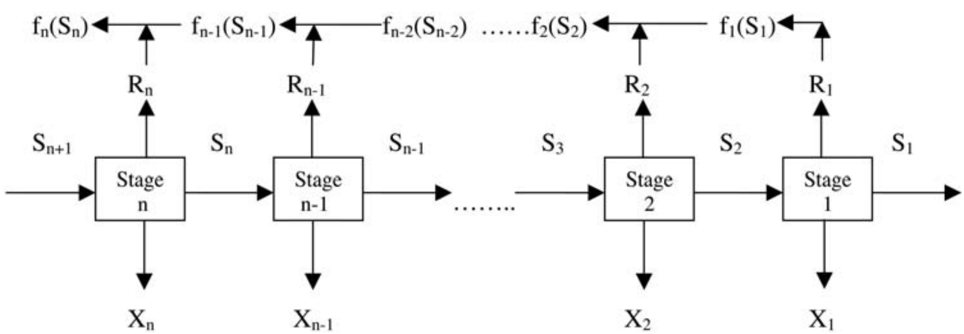

Figure 5 Dynamic process of n stages.

or design equations relate input to output and the return functions are represented as:

$$S_i = t_i(S_{i+1},\ x_i) \tag{33}$$

$$R_i = r_i(S_{i+1},\ x_i) \tag{34}$$

where x_i is the vector of decision variables at stage i.

The objective of dynamic optimization is, given the values of variables of the initial state or final state or both of the stages (boundary problem), to find the continuous decision control variable(s) that optimize some function of the individual stage returns. That is to find $x_1, x_2, \ldots, x_n$ that optimize the objective function $f(R_1, R_2, \ldots, R_n)$, mathematically expressed by:

$$f_n(S_n) = \text{opt } [R_n(S_n, X_n) + f_{n-1}(S_{n-1})] \tag{35}$$

The functions of a system may differ in nature (i.e., differential). In order for a multistage problem to be solved by dynamic programming applying the decomposition technique, the objective function must be monotonic and separable, satisfying the requirements:

$$f = \sum_{i=1}^{n} R_i = \sum_{i=1}^{n} R_i(x_i,S_{i+1})$$

$$f = \prod_{i=1}^{n} R_i = \prod_{i=1}^{n} R_i(x_i,S_{i+1}) \tag{36}$$

where x_i are real and non-negative.

4. Programming Optimization

Linear programming (LP) is an optimization method applicable to problems in which the objective function and the constraints (equalities or inequalities) appear as linear functions of the design/decision variables. Simplex method of Dantzig is the most efficient and popular method for solving general LP problems, although other superior methods as Karmarkar's have been developed. It is considered suitable for complex problems solution. In case there is a large number of variables and/or constraints, the decomposition principle can be used to solve the problem, while Karmarkar's method has been shown more efficient than the simplex method in this case.

Quadratic programming deals with problems that have a quadratic objective function, linear constraints and can be solved by suitably modifying the linear programming techniques.

If the objective function and the constraints are fairly simple, expressed in terms of the design/decision variables, the classical methods of optimization can be used to solve the problem. But classical analytical methods can not be used if the expressions are not stated as explicit functions or they are too complicated to manipulate.

Several methods are available for solving an unconstrained nonlinear optimization problem. The direct search (nongradient) methods require only the objective function values but not partial derivatives of the function in finding the optimum. The direct search (zero-order) methods use zero-order derivatives of the function. Direct methods are most suitable for simple problems involving small number of variables. The descent (gradient) techniques require, in addition to the function values, only first derivatives of the function (first-order methods) or both first and second derivatives of the function (second-order methods). Descent methods are generally more efficient than direct search techniques.

There are many techniques available for the solution of a constrained nonlinear programming problem. In the direct methods, the constraints are handled in an explicit manner, whereas in most of the indirect methods, the constrained problem is solved as a sequence of unconstrained optimization problems.

Geometric programming (GP) is a method of solving of nonlinear programming problems, where the functions and the constraints are in the form of polynomials. It places emphasis on the relative magnitudes of the terms of the objective function rather than the variables; instead of finding optimal values of the design/decision variables first, it first finds the optimal value of the objective function. Geometric programming is especially advantageous in cases that the optimal value of the objective function is of interest, as well as in optimization of a complicated problem reducing it to one involving a set of linear algebraic equations.

Many problems in plant design and operation involve variables that are not continuous but instead have integer, discrete, or fractional values. If an integer solution is desired, it is possible to use any of the common techniques and round off the optimum values of the design variables to the nearest integer values.

Integer programming (IP) refers to problems where all of the design/decision variables are restricted to be integers. A special case of IP is binary integer programming (BIP) (or zero-one programming), where all variables are either 0 or 1. Discrete programming refers to cases of problems where the variables are restricted to take only discrete values. In mixed integer programming (MIP), some of the variables are restricted to be integers while others may be continuous (fractional values). Many IP problems are linear in the objective function and constraints, hence are subject to solution by linear programming (MILP).

Stochastic or probabilistic programming deals with situations, where some or all optimization problem parameters are described by stochastic (or random or probabilistic) variables. The stochastic problem is converted into an equivalent deterministic one that can be solved by familiar techniques (linear, geometric, dynamic, and nonlinear programming).

5. Experimental Optimization—Response Surface Optimization (RSM)

In some problems when the behavior of the system or process is not known and a model cannot be developed or the model developed is very complex, experimental optimization methods are used. Experiments are designed with appropriate methods and empirical models based on the experimental data result. The optimum is then approached by using statistical techniques, the most known is the response surface method (RSM), which is widely used in food applications. Assuming that the response of *n* independent variables is a function of the levels and combinations of these variables, response surfaces that result provide insight into the overall behavior and show the existence of optimal regions.

IV. OPTIMIZATION IN FOOD EXTRACTION PROCESSING

A. Application of Optimization in Food Engineering

Optimization has been applied in several areas in food engineering, and various optimization methods have been used both in processing and manufacturing. Areas of such applications are individual equipment or total system design, process design, as well as design, layout, control, management, and operation of the total plant. Following, more details for all these application areas of optimization approaches are presented.

A selection of practical engineering perspectives referring to plant operation and optimization has been edited (13). Mathematical programming (linear, nonlinear, integer, combinatorial) and modeling techniques for various industrial applications relating to manufacturing, operation, decision-making, production scheduling, or management have been also presented (14).

Especially, optimization in design and control of chemical engineering processes approached by global optimization methods (deterministic or probabilistic) and relative applications have advanced (15). Flow-sheeting optimization during the early stages of design, applying global optimization to modular process design approaches provides many advantages (16). Genetic algorithms (GA) or evolutionary ones (EA) have been investigated in chemical engineering problems and have been proved to be powerful and robust optimizing techniques either for total processes and/or particularly for extraction processes (17, 18). Optimization resources and specific information about optimization are available on the Internet in the NEOS—Network Enabled Optimization Technology Center (OTC)—which is a joint enterprise of Argonne National Laboratory and Northwestern University (19).

The design and optimization of thermal systems is of primary interest for food engineering as is strongly related to cost as well as to food quality. Thermal processing is commonly applied in chemical processing industries and hence thermal systems are often encountered into manufacturing plants. Thermal systems are necessary in food processing plants either in thermal processes of food (pasteurization, sterilization, blanching, cooking, cooling, freezing, etc.) or in other complementary operations as storage under cooling or freezing. Consequently, thermoeconomic optimization involving thermodynamic optimization and modification of the structure and design parameters of a thermal system, allows minimization of the total cost (optimization criterion) of the system satisfying technological or environmental constraints (20).

As far as individual equipment is concerned, the design and optimization of a falling-film evaporator and the construction of a mathematical model for its operation, aiming at both minimizing the overall operating cost (by minimizing water removal cost) and maintaining product quality of a large-scale production of concentrated apple juices has been cited (21).

Optimization has found application in various processes widely used in foods, as in dehydration, heat processing, and formulation of foods. Examples of such areas where optimization techniques have been successfully used are presented.

In thermal processing of foods, the optimization problem generally consists in the determination of processing conditions, the combination of process time and retort temperature, ensuring the constraint of required safety level but simultaneously minimizing the associated quality degradation (or maximizing product quality) (22). In classic problems of thermal processed canned foods, kinetic models both of bacteria spores' inactivation and nutrients (i.e., thiamine) degradation have been proposed as basis of optimization. Optimization methods require studies of time–temperature dependent kinetics for each of these factors, or studies for finding the optimum temperature profile or the optimum container geometry of the thermally processed foods. Direct search by trial-and-error, mathematical algorithms and dynamic programming approach the optimization solution. A proper optimization technique is based on the Pontryagin's maximum principle that searches out the optimum surface temperature as a smooth, continuous function of time, which maximizes the objective function (4). Furthermore for the design and optimization of thermal processing of foods, powerful dynamic models and techniques have been developed suitable and efficient for real-time industrial applications (optimization and control), i.e., for thermal sterilization (23, 24).

As far as the food dehydration is concerned, it is related to dynamic optimization problem and the scope is to find an optimum temperature profile that would result in maximum nutrients retention (i.e., ascorbic acid) achieving the desired moisture content, given a specific drying time, while constraints for the final moisture or nutrient content of the dehydrated product may exist. Mathematical models describing the drying process of foods in accordance with the equipment used have been developed, while optimization techniques may be similar of those applied in thermal processing optimization that consider either continuous (Pontryagin maximum principle) or discrete-step optimum temperature profile (4).

Optimization is usually applied in food products formulation, as a formulation process must meet a set of specifications for nutrient levels, be cost-effective, and is subject to constraints, i.e., for combined weight or certain nutrient levels. Such problems may be solved by simple mathematical optimization technique as linear programming (25).

Optimization of the nutritional quality of formulated foods in respect to different nutrients proportions has been investigated by evaluating the effect of the component proportion in the final product nutritional quality. Therefore, it is feasible to maximize the nutritional quality of mixtures by obtaining optimum formulation or by substituting a component with another in the product formula. A usual problem is the formulation of protein mixtures intended to satisfy human requirements with respect to essential amino acids. The optimization in nutritional experiments is very significant and particularly in protein mixtures problems, because the protein quality is evaluated in vivo and it is possible to express synergism effects due to complementarities of essential amino acids. Hence, the maximum nutritional quality is desired during product development, either by changing the concentrations of the protein ingredients (soybean protein products, milk proteins, whey proteins, etc.) or by the substitution of an animal origin protein by another (vegetable or less costly) in a formulated mixture of known nutritional quality (26). In nutritional evaluation experiments the mixture response surface methodology proved to be an extremely useful tool for the optimization of the mixture's protein quality.

Moreover, the estimation of the nutrient values in commercial food products is very important for the human diet. They must be taken daily in certain quantities, some of them are essential for human health (amino acids, linoleic acid), others are functional components (dietary fibers). Many missing nutrients values for nutrients of interest are encountered in widely used foods' composition data due to lack of accepted analytical methods for some nutrients, high cost of chemical analysis, and proliferation of commercial foods. The missing nutrient value estimation is performed by various methods of different accuracy. Mathematical optimization proves more accurate to estimate nutrient values of food product than other techniques used (i.e., trial-and-error); linear programming as well as quadratic programming are comparably efficient in accuracy (27).

Sensory optimization of a food product is another application area where optimization methods have been used. The product ingredients affect many attributes of the product that determine its acceptability by the consumers. Hence, the best product formulation is found by evaluating multiple sensory attributes or responses of food, carrying different weights in the perception of the product, using graphical optimization methods (28). In product optimization problems special (classical or novel) sensory methodologies and techniques are used (29). Mathematical models with linear or quadratic equations created by experimental designs, show the relationships between independent variables (food formulas, processing conditions) and the responses (rating attributes). These models are useful for the prediction of the likely attributes, the maximization of the acceptance, or for optimization problems under certain constraints of formulation (30, 31). An example of optimizing acceptability is the case of low-calorie products containing alternative sweeteners. Following a central composite design, response surface methodology (RSM) (32) can select the optimum product formulation (optimal concentration of sweetener) that optimizes the sensory quality of the product (maximum acceptability). Also during development of new food products, combining experimental design of both product and concept generates optimal products and concept within constraints, such as cost, desired sensory profile limits, or targeted population (33).

The quality optimization of thermally processed foods (i.e., cooked) and the relative optimization methods employed for these processes are of interest in food engineering. Commercial processes try to meet the requirements for microbiological safety, nutritive value, and sensory acceptance of foods. Scope of the methods is to determine the suitable processing conditions, especially the temperature profile (temperature–time of processing), which maximize quality factors of foods undergoing thermal processing (i.e., retention or degradation of nutrients, microbial inactivation, etc.) (34).

Dried potato cubes are an example of thermally processed food, the quality of which is optimized. The process includes potato blanching in water containing pectin and polydextrose, followed by a two-step drying procedure by a batch-type high-temperature fluidized bed drier (HTFB) at varying conditions, and a tunnel drier at standard conditions. The objective is to find biopolymers concentration, time of blanching, as well as temperature and time of drying in HTFB that obtain the maximum of rehydration ratio, puffing and water holding capacity, and minimum of nonenzymatic browning (7). In such problems, RSM is usually the method used for manipulation of experimental data. Using the same technique, the extrusion of a high-protein snack has also been optimized. Maximum value of expansion ratio and sensory rating of extrudates and minimum value of shear strength was obtained by controlling the feed moisture and temperature at the central zone of the extruder barrel (7).

The optimization framework of heat-sensitive foods' drying process, being also essential for a food engineer, has been developed by combining the equipment and material models to attain the cost-effective product drying (with efficient energy saving), and minimizing its quality degradation. The potato slice is such a material that suffers from loss of quality relating to color, nutrients, taste and/or texture and therefore the optimal operation of the dryer equipment may both maximize heat recovery and minimize quality degradation (i.e., loss of ascorbic acid, nonenzymatic browning), satisfying simultaneously the imposing constraints (drying time, food moisture content, ascorbic acid content, and enzymatic browning degradation) (35).

Frying of foods is another thermal process in which the frying temperature significantly affects the quality characteristics (expansion volume, expansion ratio, color, texture parameters) and the sensory ones (appearance, texture score, acceptance score) of the fried product. As continuous process is commonly used involving certain consecutive deep frying steps, the corresponding optimum temperature values can be approached based on the quality and sensory product characteristics. A popular and effective optimization method for such multivariate problems is response surface methodology (RSM) (36).

Enzymatic synthesis processes of certain valuable compounds have increased interest for investigation of parameters affecting the enzyme-catalyzed synthesis. Enzymatic produced compounds are preferred over the chemical-synthesized products and are widely used in foods and beverages with many industrial applications, i.e., low-molecular-weight esters by lipase-catalyzed esterification are flavor compounds of commercial importance. Consequently the optimization of such enzymatic processes for economical syntheses can be attained by central composite rotatable experimental design (CCRD) using response surface methodology (RSM) to predict best performance conditions (37).

Modeling, simulation, and optimization are nowadays particularly valuable due to widespread use of computers and are important approaches to a number of problems in the food industry. Linear programming can be used for simple problems such as the optimization of product quality determining the concentrations of certain components that affect its quality. Examples of industrial processes in which linear programming has been applied are referred.

LP has been applied to optimize the fixed process arrangement in an apple juice concentration plant which includes: apple crushing, juice extraction, further pressing of the resulting pomace after rehydration, mixing of juice streams, aroma stripping (for aroma recovery), juice clarification and concentration. Optimal plant operation can maximize the net profit by arranging the operating flow rates and taking into account the effects of costs, prices, apple varieties, and the operational capacity constraints for equipment. Also, LP was utilized for quality optimization in aseptic processing, where considering the microbial and enzyme inactivation, cooking quality and component quality retention (thiamin and chlorophyll), the optimal process (holding time and temperature) was derived. Another example of optimization using LP was in potato drying, where maximizing the rate of drying and minimizing undesirable side reactions (browning, ascorbic acid oxidation) with negative effect on finished product quality, the optimal drying profile was defined. (8). In addition, LP was used to quality optimization of potato chips, where given the quality as a function of moisture content, oil content and color characteristics of chips, the optimum frying conditions (temperature and time) were determined considering the constraints for temperature, oil, and moisture content of chip, and temperature and time of frying (7).

Optimization and control by automatic systems of various food processes has been cited both for product quality and economic reasons, i.e., white wine fermentation, sugar crystallization, extrusion cooking, pasta goods production, or for other complementary industrial operations, such as collection of raw milk, reduction of product losses, and costs of water purification during cleaning in dairy industries. Optimal design and control of individual food processing equipment, i.e., climbing film evaporator for tomato juice, multistage hyperfiltration unit for apple juice is also cited (38).

Optimization of industrial operations attempts to exploit cost, time, and quality profits. For example, a methodology is proposed for optimization of a vegetable oil hydrogenation unit. A mathematical model based on data from a hydrogenation plant is developed to select the optimum operating conditions of temperature and hydrogen pressure that provide the desired product in minimum time (39).

On the other hand, optimization of the overall efficiency, total operating cost, yield, total return, quality of output, and throughput of the whole food manufacturing plant is necessary when changing the raw materials or the product properties. Of course, it can be applied to large food processing plants; it is evident that routine application of optimization methods during operation is practiced only in certain parts of industrial plants. However, with the increased use of computers and computer control in food manufacturing integrated optimization may be applied to every modern processing plant. The new approach for food process and plant optimization is optimization throughout the food chain. The optimization of a complete food chain consists of product, process, and raw materials optimization, and by analyzing the system efficiency (losses, wastes) leading to optimum plant, process, and equipment design and operation (40).

Finally, optimization is also applied in management and control of food processing plants. Application of optimization in management of food processing and food service industries has been presented.

In addition to the above applications of optimization in food processing, similar techniques are used in optimizing food analysis methods of high accuracy such as gas and liquid chromatographic methods (41). This has increased significance when the constituents of interest are related to food safety specifications. Also, optimization of instrumental measurements related to foods have been investigated, i.e., methodologies for extracting features from sensors output responses of instrument analyses (electronic nose, near infrared analyzer) (42, 43).

In conclusion, it is clear that the increased use of optimization in food manufacturing enables the efficiency, productivity, and quality to be increased and the energy use, product loss, and environmental pollution to be reduced. Furthermore, the optimization philosophy, ideas, and techniques should be adopted throughout the food handling system—from the harvesting of raw materials to the transportation, processing, packaging, distribution, and consumption of the final products.

B. Optimization of Extraction Processes

Extraction is applied to recover or remove constituents and consequently the product of interest may be the extracted materials or the extracts. The design and optimization of an extraction process entails the knowledge and the role of the technological parameters of the process.

Conventional solvent extraction involves the removal of certain constituents from a mixture of solids (leaching or solid extraction) or liquids (liquid extraction) by means of a solvent in which exhibit different solubility. Supercritical fluid extraction (SFE) involves the separating of a mixture by contacting it with a fluid under conditions of temperature and pressure above its critical point. The separation of solvent from the extracted solute in conventional extraction is carried out by distillation or evaporation, while in SFE separation is accomplished either by reducing the pressure at constant temperature or by raising the temperature at constant pressure (44). Following, the most important parameters that significantly affect the extraction efficiency and determine the process design and success are presented.

In leaching, the important parameters are:

1. The preparation of solid material by size reduction (crushing, grinding, flaking or cutting into pieces or cosettes); solid size must be suitable (surface area per unit volume) to make the solute more accessible to the solvent and to favor the extraction but not very fine to cause packing of solids and impede free flow of solvent
2. The selection of solvent for extraction based on a number of characteristics (capacity, selectivity, chemical inertness, thermophysical properties, flammability, toxicity, cost, availability)
3. The selection of operating temperature—temperature must be high enough to give higher solubility of solute in solvents, but not very high to cause solvent losses, extraction of undesirable constituents or damage of sensitive components
4. The equipment depending on the mode of operations (batch or continuous), the solids handled (fixed bed, percolation, full immersion, intermittent drainage or dispersed/moving contact) or the performing arrangement (one stage or multistage)

In liquid extraction the important parameters are:

1. The selection of solvent as previously referred, mainly based on high solute capacity and selectivity; particularly, solvent interfacial tension must have low value to get a good dispersion with high interfacial area for extraction, but not very low to cause emulsion formation and create problems in separation
2. The equipment depending on the contacting of the phases (by gravity or by centrifugal force)

In supercritical fluid extraction the important parameters are:

1. The capacity and selectivity of the extracting supercritical fluid and their dependence on temperature and pressure
2. The ratio of solvent mass flow rate to the mass of solids treated; knowledge of the solvent, raw material and extract physical properties is necessary
3. The operating pressure and temperature, which must not cause decomposition of the raw material
4. Bulk density of the solid feed depending on the density of the solids, the form and consistency of the material and its moisture content
5. The mechanical treatment of the raw material depending on the nature of raw material (raw material purification or extract recovery); mechanical treatment should be avoided in the case of solids recovery, whereas in the production of a soluble extract may be desirable
6. The time of extraction in respect to solvents, raw material feed and operating conditions

The technical and economical feasibility of an extraction process is determined knowing the equipment size, operating conditions, solvent flow rates and extraction yields. Extraction optimization is involved both in the design and the operating conditions for the equipment (separation allocation, differences in physical and/or chemical properties for separation, equipment type and sequence separators, fixation of separated phases, entire process operating conditions).

Optimization of liquid–liquid extraction processes has been investigated and examples for staged and continuous models of extraction appeared in the literature (45). In staged processes treated as an integer variable, the optimization is more difficult, while in continuous processes for either cocurrent or countercurrent flow, integer variables are avoided and optimization can be carried out by other techniques. Steady-state continuous countercurrent liquid extraction has been modeled; a plug flow model was proved sufficiently accurate for a continuous pilot-scale extraction column. It can be used to determine the maximum extraction rate to various applications.

A common problem in optimization of extraction processes is that operation time for the lowest cost is usually different from the time that gives the best yield (effectiveness), so that it is impossible to have both optimal cost and yield simultaneously. In this case the operation time becomes the independent parameter whose value determines the value of the criteria: minimum cost and maximum yield. The relative importance of the two conflicting criteria must be judged in order to obtain an optimum extraction time. So, if lowering of the operation cost is of interest, the time of extraction will be optimized, while the yield will be the primary criterion in an isolation of desired components or removal of toxic substances from food sources. Suboptimum with respect to operation cost and yield or optimum with respect to the combined criteria of cost and yield may be found. An overall criterion function can be established applying a more formalized optimization. Regional constraints on time might be imposed; a very large time above a certain value is not cost effective or the yield is not accepted at time below a certain value. After the optimum operation time has been determined other parameters not included in the original problem (extraction medium, extraction system) may be used, thus decreasing the operation cost and increasing yield by formal optimization techniques. It must be noted that formal optimization theory should be used only to find optimum parameters in well-defined systems with quantitative-dependent and independent parameters, criterion function, and functional and regional constraints.

C. Application of Optimization in Food Extraction Processing

Extraction is a separation process widely used in food processing industry for various applications, while recently with supercritical fluid extraction is possible to improve the quality of food products. Extraction may be a basic step in processing of many food products (i.e. sugar, edible oils, etc.), used for the recovery of active constituents or for the removal of undesirable constituents from raw materials, while important components may be separated from natural products with many applications to food industries (flavors, antioxidants, etc.).

Optimization of protein isolation process by optimizing the protein extraction step has been studied from oilseeds or beans as: tomato seed, pigeon pea, peanut, and flaxseed (46, 47, 48, 49). The protein isolation process from vegetable sources includes mainly extraction or leaching of proteins by aqueous solutions and isoeletric precipitation; therefore extraction of proteins, evaluated by protein extraction yield, is determinant for the total protein yield of the whole protein isolation process. The optimization of this process should attain the maximum both of protein extraction yield or total protein yield as well as of the protein quality of the isolated product. It must be mentioned that the conditions optimizing the above responses are not the same; usually maximizing the protein extraction yield or the total protein yield decreases protein isolate content. Thus, the basic factors affecting protein solubilization during extraction such as: particle size of proteinaceous material, temperature, extracting medium (water or diluted salt solution), solid to liquid ratio, pH (neutral or alkaline region) have been studied by proper experimental design and using response surface methodology (RSM) or steepest-ascent gradient method. Mathematical models for the protein extraction yield or total protein yield as well as for the protein content of protein isolate were obtained, while the extraction conditions that lead to the maximization of the responses were determined.

Surimi usually used as raw material in processed foods (fish sausage, fish cake, or kamaboko) is water-leached, minced flesh of deboned fish. Surimi processing starts with leaching and additional processes follow, such as grinding, setting, heating, and frozen storage. Because the processing conditions significantly affect the quality characteristics of surimi products (gel strength, whiteness) the optimization of surimi processing should be conducted. An optimization study has been presented that uses a surface response method with a central composite design of surimi processing experimentation. Among the processing conditions the leaching parameters (leaching water in each leaching cycle, number of leaching cycles) were examined as well as parameters of the following processing steps. The optimal processing conditions that maximize gel strength and minimize whiteness of surimi products by canonical analysis and ridge analysis as well as fitting of a suitable model was investigated (50).

Optimization has been widely applied to oil processing industry, in oil solvent extraction as well as in oil expression or mechanical extraction.

Mechanical extraction is an alternative method for oil expression by crushing the seeds in a mechanical screw press. In this case, both oil yield and energy pressing cost are affected by the preprocessing conditions of the seed (dehulling, preheating, flaking or grinding, seed moisture content, seed temperature prior of pressing) as well as by the design and operation characteristics of the press (pressure, temperature, pressing time) and their interactions. Mathematical models based on expression conditions have been developed to predict the maximum sunflower oil recovery (51).

Olive oil is characterized as a "natural food product" because it is the only oil produced by mechanical method that can be consumed without further processing. In addition, due to its nutritive and health properties, olive oil is recognized as a functional food product. This oil, virgin olive oil, should meet certain specifications according to regulation EC No. 2568/91 related to quality characteristics (oil acidity or oxidative status, etc.). For the above reasons, special mechanical methods have been developed. The classical method of extraction of olive oil is based on the mechanical pressing of olives. An alternative method also has been developed, which involves centrifugal separation of olive oil using horizontal decanters. Special quality levels can be attained in virgin olive oil production when all operations (olive collection and storage, extraction processing, packaging and storage of end product) are carefully carried out.

Efficiency of expression is usually evaluated by extraction yield expressed as percent of oil extracted to the percent of oil in the olives. The expression parameters affecting oil yield have been examined: pressure compaction rate, cake thickness, rigid solid (pits) content in the olive paste, and the optimization of olive paste expression process has been studied experimentally (52). Consequently, the simultaneous variation of the parameters must be investigated to obtain the maximum olive oil extraction yield and the optimal operation of industrial olive pressing systems to be determined. The pressure raise increases oil yield, however it is important for olive oil quality the pressure to be kept under constrained values. Therefore, the effect on olive oil quality of parameters, such as olive ripening and storage prior to processing and olive paste mixing time and temperature, should be studied so extraction can be optimized for oil quality requirements (53).

In recent years, extraction of vegetable oils using supercritical fluid extraction (SFE) as an alternative to the current industrial processes (expeller pressing, solvent extraction) and its optimization has been investigated (54, 55). Carbon dioxide, which is the most commonly used solvent to SFE processes, is also used in oil extraction; supercritical pentane has also been cited (54). The efficiency of SFE of oils depends on the variables: temperature, pressure, particle size of seeds, contact time between the extracting fluid and the oil-bearing material, ability of the fluid to penetrate the oil-bearing material, and solubility of the oil in the extracting fluid. Optimization of SFE of various vegetable oils such as soybean oil, canola oil, and sunflower oil, has been studied and the conditions that maximize oil recovery have been determined. In particular, the effect of extraction variables on oil recovery has been estimated by factorial designs and the optimum extraction conditions have been found using modified simplex method for the case of soybean oil. Simulation and modeling of a sunflower oil SFE plant and the optimization of the continuous process operation (extraction and CO_2 recovery) was carried out and the optimal operating conditions found (55). Mathematical model of a fixed-bed extractor of canola oil has been presented giving the concentration of oil on both the solid and fluid phases and determining the overall volumetric mass transfer coefficients; a one-dimensional unsteady state model was used and the predicted results were in good agreement with the respective experimental results (56).

Extractive processes used in alcoholic food/beverage products have been studied and optimized. The design, optimization, and control of extractive alcoholic fermentation in continuous mode are preferred. Combined with selective ethanol extraction, fermentation is enhanced; the combination of fermentation and selective ethanol extraction enables efficient control of the process. The dynamic behavior of the process was studied by factorial design simulating industrial process, and a dynamic matrix control (DMC) algorithm was used to control the extractive process. Modeling and simulation with response surface analysis was used to determine the operational conditions that maximize alcohol yield and productivity (57). Also, a countercurrent supercritical fluid extraction process on a pilot plant of distilled alcoholic drinks has been studied to optimize the efficiency of ethanol extraction yield. Thus, by factorial experimental design the extraction and fractionation conditions determined the ethanol percentage and the total yield of extracted ethanol of the residual extracted drink and of each isolated fraction, allowing the production of concentrated extracts with a rich aroma and low ethanol content (58).

Other analytical extractive processes that have been optimized are the separation of certain amino acids (i.e., DL-tryptophan), which are important food components from aqueous solution using an emulsion liquid membrane. The critical extraction parameters: carrier concentration in the membrane system, pH, initial amino acids concentration were studied and using response surface methodology (RSM) the optimum separation conditions were found where the maximum amino acid extraction yield was attained (59).

Extraction (or acid leaching) is a special step or pretreatment in many cases of analytical procedures of some determinations in food matrixes: vitamins, trace elements, pesticides residues, etc., in foods, industrial products, water, or soil. The analytes should be isolated and/or preconcentrated without changing their original chemical forms and subsequently analyzed using analytical or instrumental methods (i.e., atomic absorption spectrometry in trace elements, chromatographic methods such as gas chromatography (GC), high-performance liquid chromatography (HPLC) in pesticides or vitamins, spectrophotometry in tannins, etc.). The optimization of an analytical procedure often involves the study of the effects of experimental conditions particularly of time consuming and expensive ones as the extraction pretreatment processes (60–66). Critical variables in such extraction (or leaching) procedures are: type of solvent (organic solvent, saponification reagent, acid/oxidant reagent type and concentration), leaching volume, time, temperature, particle size of ground food product (matrix), extraction method. The particular variables relative to the extraction method are: (a) soxhlet: reflux frequency; (b) solid-phase extraction (SPE): type of sorbent, eluting solvent flow rate, sample pH, sample volume, elution volume, addition of modifier, water sample flow rate; (c) supercritical fluid extraction (SFE): CO_2 pressure, temperature, static, and dynamic time; and (d) ultrasound or microwave assisted: sonication, frequency of ultrasound energy or microwave power, exposure time, temperature (67, 68). Experimental (central composite, Plackett-Burman—PBD, orthogonal array—OAD) design and simplex optimization method or response surface methodology (RSM) are effectively used to study the effects of extraction variables and find the optimum values of extraction variables in which maximum percent recovery of the extracted components is attained.

NOMENCLATURE

$x_i(i = 1, 2, \ldots n)$	independent parameters, variables, design variables in optimization problem
$x, (x_1, x_2, \ldots\ldots, x_n)$	vector of *n* variables, n-dimensional vector, design vector
X	matrix
X_{ij} or x_{ij}	elements of matrix X
x^*	extremum (minimizer/ maximizer)
$x = [x_1, x_2, \ldots\ldots, x_n]^T$	column vector
$x^{(k)}, \{x^{(k)}\}\ k = 1, 2, \ldots$	iterates in an iterative method
$f(x), f(X)$	objective function
$h(x), h_j(X)$	vector of equality constraints
$g(x), g_j(X)$	vector of inequality constraints
$C, f(x_1, \ldots, x_n)$	optimization criterion function
$fc_i = f_i(x_1, x_2, \ldots\ldots, x_n)$	functional constraints
$l_1 \le r_i(x_1, x_2, \ldots\ldots, x_n) \le l_2$	regional constraints
$f'(x)$, dx	first derivative of function
$f''(x)$	second derivative of function
$d^r f(x)$	rth differential of f(x) (partial derivative of r order)
$\nabla f(x)$	first partial derivative or gradient vector
$\nabla, (\partial f/\partial x_1, \partial f/\partial x_2, \ldots\ldots, \partial f/\partial x_n)^T$	first derivative operator (elements $\partial x_i/\partial x_j$)
$\nabla^2 f(x)$	second partial derivative
∇^2	second derivative operator (elements $\partial^2/\partial x_i\,\partial x_j$)
$H(x), \nabla(\partial f/\partial x_j), \nabla(\nabla f^T)$	Hessian matrix
$J\big\|_{x=x^*} = [\partial^2 f/(\partial x_i\,\partial x_j)\big\|_{x=x^*}]$	Hessian matrix of f(X)
$d^k\big\|_{x=x^*}$	k-order differential of f at X*
$J\left(\dfrac{f, g_1, g_2, \ldots, g_m}{x_k, x_1, x_2, \ldots, x_m}\right)$	Jacobian determinants
L	Lagrange function
λ_j	Lagrange multipliers
R^n	*n*-dimensional space
BIP	binary integer programming
CCD	central composite design
CCRD	central composite rotatable design
GMP	geometric programming

IP	integer programming
LP	linear programming
MILP	mixed integer linear programming
MIP	mixed integer programming
NLP	nonlinear programming
OAD	orthogonal array design
PBD	Plackett-Burman design
RSM	response surface optimization
SFE	supercritical fluid extraction
SPE	solid-phase extraction

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