EXPERIMENTAL DESIGN OPTIMIZATION AND THERMOPHYSICAL PARAMETER ESTIMATION OF COMPOSITE MATERIALS USING GENETIC ALGORITHMS

by

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Experimental Design Optimization and Thermophysical Parameter Estimation of Composite Materials Using Genetic Algorithms

Sandrine Garcia

(ABSTRACT)

Thermophysical characterization of anisotropic composite materials is extremely important in the control of today fabrication processes and in the prediction of structure failure due to thermal stresses. Accuracy in the estimation of the thermal properties can be improved if the experiments are designed carefully. However, on one hand, the typically used parametric study for the design optimization is tedious and time intensive. On the other hand, commonly used gradient-based estimation methods show instabilities resulting in nonconvergence when used with models that contain correlated or nearly correlated parameters.

The objectives of this research were to develop systematic and reliable methodologies for both Experimental Design Optimization (EDO) used for the determination of thermal properties, and Simultaneous Parameter Estimation (SPE). Because of their advantageous features, Genetic Algorithms (GAs) were investigated for use as a strategy for both EDO and SPE. The EDO and SPE approaches used involved the maximization of an optimality criterion associated with the sensitivity matrix of the unknown parameters, and the minimization of the ordinary least squares error, respectively. Two versions of a general-purpose genetic-based program were developed: one is designed for the analysis of any EDO / SPE problems for which a mathematical model can be provided, while the other incorporates a control-volume finite difference scheme allowing for the practical analysis of complex problems. The former version was used to illustrate the genetic performance on the optimization of a difficult mathematical test function.

Two test cases previously solved in the literature were first analyzed to demonstrate and assess the genetic-based {EDO/SPE} methodology. These problems included the optimization of one and two dimensional designs for the estimation at ambient temperature of two and three thermal properties, respectively (effective thermal conductivity parallel and perpendicular to the fibers plane and effective volumetric heat capacity), of anisotropic carbon/epoxy composite materials. The two dimensional case was further investigated to

evaluate the effects of the optimality criterion used for the experimental design on the accuracy of the estimated properties.

The general-purpose genetic-based program was then successively applied to three advanced studies involving the thermal characterization of carbon/epoxy anisotropic composites. These studies included the SPE of successively three, seven and nine thermophysical parameters, with for the latter case, a two dimensional EDO with seven experimental key parameters. In two of the three studies, the parameters were defined to represent the dependence of the thermal properties with temperature. Eventually, the kinetic characterization of the curing of three thermosetting materials (an epoxy, a polyester and a rubber compound) was accomplished resulting in the SPE of six kinetic parameters.

Overall, the genetic method was found to perform extremely well despite the high degree of correlation and low sensitivity of many parameters in all cases studied. This work therefore validates the use of GAs for the thermophysical characterization of anisotropic composite materials. The significance in using such algorithms is not only the solution to ill-conditioned problems but also, a drastically cost savings in both experimental and time expenses as they allow for the EDO and SPE of several parameters at once.

Keywords : Anisotropic Composite Materials - Experimental Design Optimization - Genetic Algorithms - Kinetic Parameters - Parameter Estimation - Thermal Properties - Thermosetting Materials.

Conception Optimale d'Expériences et Estimation de Paramètres Thermophysiques de Matériaux Composites par Algorithmes Génétiques

Sandrine Garcia

(RESUME)

La caractérisation thermophysique de matériaux composites est un enjeu crucial. La précision de l'estimation peut être améliorée si les expériences sont conçues avec pertinence. Cependant, l'étude paramétrique traditionnellement employée pour l'optimisation expérimentale est limitée, et les méthodes d'estimation basées sur le calcul d'un gradient sont instables pour des problèmes mal conditionnés.

L'objectif de ce travail était de développer des méthodologies robustes pour la Conception Optimale d'Expériences (COE) destinées à l'identification de propriétés thermiques, et pour l'Estimation Simultanée de Paramètres (ESP). L'approche utilisée s'appuie sur les spécificités avantageuses des Algorithmes Génétiques (AGs) et consiste en COE à maximiser un critère d'optimisation basé sur la matrice de sensibilité des propriétés recherchées et en ESP, à minimiser l'erreur des moindres carrés. Un programme général basé sur les AGs a été développé sous deux versions, permettant l'analyse soit de modèles analytiques soit de modèles numériques par volumes finis.

Les AGs de COE et d'ESP ont d'abord été testés sur des cas de la littérature, puis appliqués sur des cas nouveaux. Ces études ont été menées selon une approche à la fois numérique et expérimentale. Elles concernent la caractérisation thermique de composites anisotropes carbone/époxy, avec des COE et ESP comportant respectivement jusqu'à sept paramètres expérimentaux, et neufs paramètres thermophysiques. Enfin, la méthodologie d'ESP a été étendue à la caractérisation de cinétiques chimiques de résines thermodurcissables mettant en jeu six paramètres cinétiques.

Malgré de très fortes corrélations et faibles sensibilités de plusieurs paramètres dans toutes les études, les résultats confirment la remarquable robustesse des AGs. L'intérêt de leur utilisation réside non seulement dans la solution de problèmes mal posés, mais aussi dans la réduction de temps et coûts expérimentaux, en permettant des estimations simultanées de plusieurs paramètres.

Mots Clefs : Algorithmes Génétiques - Cinétiques Chimiques - Conception Optimale d’Expériences - Matériaux Composites Anisotropes - Méthodes Inverses - Propriétés Thermophysiques - Résines Thermodurcissables - Sensibilité et Corrélation.

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List of Symbols

A_1, A_2	Arrhenius constants (min^{-1})
b	Estimated parameter vector using the Gauss linearization method
B	Parameter of the inhibition time model
C_p	Specific heat (J/kgK)
C	Volumetric heat capacity, (ρC_p, J/m^3K)
CRITERION	Variation Size to be checked in the convergence criterion (used in the GA_3)
d	Element of the $\mathbf{X}^T\mathbf{X}$ matrix
D	Determinant of the $\mathbf{X}^T\mathbf{X}$ matrix
E_1, E_2	Arrhenius constants or activation energy constants (kJ/mole)
f	Fitness of a chromosome
f_{eval}	Number of function evaluation
f6	Mathematical test function
h	Scalar interpolation factor in the modified Box-Kanemasu method
h_1, h_2, h_f	Convection coefficients used in Section 5.2.2 (W/m^2K)
$h(t,T)$	Integral function used in the inhibition time model (s)
$h(t)$	Enthalpy function (J/s)
ΔH	Total heat of reaction (J)
i, j	Node position along the x- and y-axis, respectively (numerical model)
k	Thermal conductivity (W/mK)
k_x	Thermal conductivity perpendicular to the fiber plane (W/mK)
k_y	Thermal conductivity parallel to the fiber plane (W/mK)
K_1, K_2	Kinetic rate constants (min^{-1})
L	Length (m)
L_p	Heating length (m)
LASTG	Maximum allowable number of generations
LASTCRITERG	Number of generations during which the convergence criterion must be satisfied for the run to stop (used in the GA_3)
MING	Number of generations without checking the convergence criterion (used in the GA_3)
m, n	Kinetic exponents
n_{best1}, n_{best2}, n_{best3}	Elitist genetic parameters used in the EEGA
n_{pop}	Number of initial population investigated with the EEGA
n_g	Number of generations
n_p	Number of parameters
n_s	Population size
N_i	Number of observations (per experiment / sensor)
N_j	Number of experiments
N_k	Number of sensors
N_{tot}	Total number of observations
p	Probability
p_c	Probability used in the crossover (genetic operator)
p_{mj}	Probability used in the jump mutation (genetic operator)
p_{mc}	Probability used in the creep mutation (genetic operator)
p_r	Probability used in the generational replacement (genetic operator)

p_t	Probability used in the tournament selection (genetic operator)
$\mathbf{P}$	$[\mathbf{X}^T\mathbf{X}]^{-1}$ with OLS estimator
q	Heat flux (W/m^2)
r	Correlation term
R	Random number uniformly distributed between 0 and 1 [Chapter 4] Gas constant (kJ/mole-K) [Chapter 6]
R_c	Contact resistance (m^2K/W)
s	Sample standard deviation around the mean
s_i	Sample standard deviation of an individual experiment
S	Least squares function
S_1, S_2, S_3	Least squares function associated with Strategies I, II and III, respectively
t	Time (s)
t_n	Total overall experimental time (s)
t_h	Heating time (s)
t_{12}	Cooling time optimized in Section 5.2.1 (s)
t_{ref}	Parameter of the inhibition time model (s)
T	Temperature (°C or K)
T_{ref}	Reference temperature selected in the inhibition time model (s)
$\mathbf{U}$	Matrix used with MAP estimator
v	Rate of cure ($d\alpha/dt$, min^{-1})
V_f	Fiber volume fraction
V_T	Temperature rate imposed in DSC experiments (°C/min)
$\mathbf{W}$	Weighted matrix used with ML and MAP estimators
x	Location on x-axis
X	Sensitivity coefficient
$\mathbf{X}$	Sensitivity matrix
$\mathbf{X}^T\mathbf{X}$	Fisher information matrix
y	Location on y-axis

Greek

α	Thermal diffusivity (m^2/s) [Chapter 5]; Degree of cure [Chapter 6]
$\boldsymbol{\beta}$	True parameter vector
δ	Perturbation size
Δ	Step/Variation
η	Dependent variable (measured quantity in estimation procedure)
$\boldsymbol{\eta}$	Observation vector
κ_{xy}	Ratio of thermal conductivities k_y/k_x
λ	Eigenvalue of the $\mathbf{X}^T\mathbf{X}$ matrix
$\boldsymbol{\mu}$	Prior information parameter vector
ρ	Density (kg/m^3)
σ	Standard deviation

Superscripts

$+$	dimensionless
$\tilde{}$	experimental
$\bar{}$	mean

k	iteration
f	fiber or fluid
m	matrix

Subscripts

a	ambient
av	average
eff	effective
i	initial
ind	induction
max	maximum
min	minimum
p	plate
ref	reference
s	sensor

List of Abbreviations

ALIS	Laboratory Apparatus from ISitem
CIs	Confidence Intervals
EDO	Experimental Design Optimization
BEGA	Basic Elitist Genetic Algorithm
DSC	Differential Scanning Calorimetry
EEGA	Extended Elitist Genetic Algorithm
GA_3	Third Genetic Algorithm (2 versions: GAMAIN and GACONDUCT)
GAs	Genetic Algorithms
K&S	Kamal and Sourour (kinetic model)
LTI	Laboratoire de Thermocinétique de l'ISITEM
MAP	Maximum A Posteriori (estimator)
ML	Maximum Likelihood (estimator)
OLS	Ordinary Least Squares (estimator)
RMS	Root-Mean-Square error
RTM	Resin Transfer Molding
SPE	Simultaneous Parameter Estimation
TC	Thermocouple
VT	Virginia Tech (Virginia Polytechnic Institute and State University)

CHAPTER 1

Introduction

1.1 Motivation

Composite materials can offer superior performance over standard metals, including higher strength-to-weight ratios and better corrosion and wear resistance. Because of these improved characteristics the use of these materials has been growing rapidly in this past quarter century. Composite technology prevails in a wide variety of fields, including the aerospace, aeronautics, automotive, tooling and sporting goods industries, to name but a few. In these high technology applications it is important that the properties of these advanced materials be known for design purposes. Knowledge of the thermal properties is particularly important in modeling composite fabrication processes and in predicting thermal stresses developed when the materials are subjected to non-isothermal environments. On the one hand, composite fabrication processes involve high coupling between heat transfer within the material and exothermic chemical reactions. The control of these thermal phenomena is a crucial aspect for improvement in productivity and quality of components. Such control requires the ability to simultaneously predict both the temperature distribution within the material and the rate of cure. This necessitates the knowledge of both the thermal properties and the parameters of the kinetic model governing the curing process. On the other hand, thermal stress analysis is essential in the design of aerospace structures and vehicles, as these structures undergo extreme and dynamic thermal conditions. The thermal loads applied on the materials induce large temperature gradients within the structure, which in turn result in the development of thermal stresses and thus possible structural failure. To prevent this, the temperature response of the structure to an applied heat flux must be investigated, which necessitates knowledge of the thermal properties.

The thermal properties necessitated in both fields of study described above include the effective conductivity and volumetric heat capacity. These properties are thermally dependent and due to the anisotropic characteristic of composite materials the conductivity is also directionally dependent. Composites with polymeric matrix and unidirectional fibers are considered in this work. Two conductivity components, parallel and perpendicular to the fiber plane, thus govern conduction within the material. Many experimental and analytical methods have been proposed for determining these thermal properties. An alternative is to use a parameter estimation procedure that consists of the minimization of an objective function, and that allows for the simultaneous estimation of the thermal properties. The objective function usually contains the sum of squared error between measured and calculated temperatures from a mathematical model. Experiments are therefore required with this approach.

The accuracy of the estimated properties is directly related to the sensitivity of the temperature distribution with respect to the thermal properties and can be increased if the experiments are carefully designed (Beck and Arnold, 1977). Experimental parameters such as sensor location, heating time, and heating area are important factors to be considered in the design. Optimization of experimental designs used in the prediction of thermal properties is therefore crucial in maximizing the amount of information that can be obtained from the experiments. The optimal input conditions are typically found by maximizing a single criterion associated with the sensitivity matrix of the unknown properties to be estimated. Among the different design criteria, the *D*-optimality criterion is the most commonly used and is often recommended because it allows thermal property estimates to be obtained with minimum variances. Due to the complexity of an analytical scheme in most cases, the optimization technique typically applied is a stepwise parametric study. However, because it is an iterative process, this technique is tedious and time intensive and therefore restricts the researchers from expanding their work to the optimization of a large number of design variables (e.g. more than three) and to complex designs. In addition to its lack of efficiency, the parametric study does not guarantee the determination of global optima.

The optimal designs are then used in a parameter estimation procedure. Commonly used procedures involve the computation of the gradient. One recommended procedure (Beck and Arnold, 1977) is the modified Box-Kanemasu method that has proven to be effective provided there is sufficient information from the sensitivity coefficients of the unknown thermal properties, and no correlation between the properties. Generally speaking, two parameters are considered correlated when their sensitivity coefficients are nearly (more than 90% as a rule of thumb) linearly dependent. The modified Box-Kanemasu method is a modification of the

Gauss method, which is a first-order unconstrained descent method. However, when used with models that contain correlated or nearly correlated properties, the modified Box-Kanemasu method can show instabilities resulting in non-convergence. Indeed, correlation or near-correlation among parameters is known to be a limiting factor for the converged application of gradient-based estimation procedures. One difficulty in the simultaneous estimation of both directional thermal conductivities of composite materials is that these parameters are correlated. Typically, the approach is, therefore, to first determine the component orthogonal to the fibers using measurements from a specific experimental design and then to assume this property known to estimate the component in the transverse direction using another design.

Correlation is also encountered among the parameters of the kinetic model governing the curing during composite material processing. These parameters usually involve one or two rate constant(s) which follow an Arrhenius law, and one or two exponent(s). Application of gradient-based procedures for the simultaneous estimation of the kinetic parameters is therefore restricted to the identification of the uncorrelated parameters assuming the others to be known.

The need for systematic and reliable methodologies for both (1) Experimental Design Optimization (EDO) used in the determination of thermal properties, and (2) Simultaneous Parameter Estimation (SPE), provided the motivation for this research. The driving force was on developing EDO and SPE procedures that overcome the limits of commonly used ones, parametric studies and gradient-based methods, respectively. Primary efforts were focused on selecting an optimization/estimation method that could efficiently search a multimodal parametric space for a global optimum. The three main types of search methods include calculus-based methods, enumerative techniques and random/probabilistic search algorithms. The first and second type were eliminated as they involve methods that present the same attributes (and therefore same limits) as gradient-based methods and parametric studies, respectively. Methods from the third type, and more particularly those presenting the attribute of probabilistic evolutionary search, have actually achieved increasing popularity as researchers have recognized the shortcomings of the two previous types. Besides their non-gradient nature, their main advantages encompass the ability to avoid local optima and to handle complex non-linear objective functions while being straightforward to apply. Genetic Algorithms (GAs), which belong to the field of evolutionary computation, are based on

genetic and selection mechanisms of nature, and provide for the minimization of an objective function using a probabilistic directed search without the use of derivatives. These algorithms have been theoretically and empirically proven to provide robust searches in complex spaces (Goldberg, 1981), and in this last decade, have shown their effectiveness and efficiency in the engineering field. Because of their advantageous features, GAs were investigated for use in this study as a strategy for both EDO and SPE. The motivation in using GAs was their potential to overcome both the lack of efficiency of parametric studies, and the restriction to the estimation of non-correlated parameters of gradient-based methods, as introduced earlier. Note the originality of this research as there is no knowledge of previous work done with GAs in the field of the thermophysical characterization of anisotropic composite materials.

This work is associated with a dual US-French PhD program between the Department of Mechanical Engineering at Virginia Tech (VT), USA, and the Laboratoire de Thermocinétique de l'ISITEM (LTI) of the University of Nantes, France. The project was initiated at VT as part of a multi-year research cooperation with the Thermal Structures Branch of NASA Langley Research Center, Hampton, VA, USA. The goal of this cooperation, which started in 1993 and ended in 1998, was to develop methodologies for the Thermal Characterization of Aerospace Structures. The strategy used in this multi-year research effort was to first develop methodologies for relatively simple systems and then to systematically modify these methodologies to analyze complex structures. This can be thought of as a building block approach. This work was built upon the previous analysis performed by Moncman (1994) and Hanak (1995). (Also note Moncman et al., 1995). Moncman developed experimental designs for the estimation of thermal properties of composites subjected to one-dimensional heat transfer. Hanak focused on two-dimensional designs and on the experimental verification of these designs. This latter work emphasized the limits of the traditionally used techniques in both design optimization and thermal property estimation. By overcoming these limits, the contribution of this investigation will enable instrumentation of a complex structure and simultaneous acquisition of meaningful property data.

The second stage of this dual program was performed at the LTI in Nantes. The project was incorporated into the applications of the research Group "Thermique des Matériaux et des Procédés de Mise en Forme" (*Thermal Analysis of Materials and of Fabrication Processes*), the goal of which is to analyze inverse problems associated with thermal effects in composite material fabrication processes. The development of genetic-based EDO and SPE

methodologies were thought here to contribute to both the thermal characterization of composite materials and the kinetic characterization of curing processes for the control of composite fabrication processes.

1.2 Goals and Objectives

The overall goals of this research were divided into two major areas:

I. the development of an Experimental Design Optimization methodology for thermal property estimation,

and,

II. the development of a Simultaneous Parameter Estimation methodology for general use.

The emphasis was on formulating sufficiently general and robust approaches allowing for practical applications of the methodologies. In order to achieve these goals, a generalized genetic-based methodology was developed for both areas of interest.

Specific short-term objectives were formulated and are:

1. develop an optimization code based on GAs and validate the optimization methodology on test problems;
2. expand the GA code to include an estimation procedure and validate the estimation methodology on test problems, in particular problems involving correlations among the properties to be estimated;
3. analyze the effects of the optimality criterion in terms of the consequent accuracy of the thermal property estimates;
4. formulate the GA code as a general-purpose computer program for the analysis of any mathematical model; demonstrate its performance on a mathematical test function given in the literature and investigate the effects of genetic operators in terms of convergence of the algorithm;

and,

5. extend the optimization/estimation methodology to a variety of optimal design and simultaneous parameter estimation problems.

The first two objectives were directed towards the appraisal of using GAs as both EDO and SPE methodologies. First, a standard GA with real-number coding and featuring a Basic Elitist strategy (BEGA) was developed for the optimization of experiments. The optimization methodology was demonstrated and verified using two test cases previously solved in the literature using a parametric study. The experiments investigated included one- and two-dimensional optimal designs performed by Moncman (1994) and Hanak (1995), respectively, for the estimation of thermal properties of composite materials. In the first case, sensor location and heating time were optimized for the simultaneous estimation of the effective thermal conductivity through the fiber plane and the volumetric heat capacity. In the second case, four parameters involving sensor location, heating time and heating area, were optimized in experiments used to simultaneously estimate both effective thermal conductivities perpendicular and parallel to the fibers and the volumetric heat capacity. In both cases, the experimental design was optimized by maximizing the objective function based on the *D*-criterion. To improve the computational efficiency of the BEGA, particularly for expensive objective functions, the algorithm was modified to form an Extended Elitist GA (EEGA). The EEGA was applied to the two test cases discussed above, and the performance of the EEGA was compared with the results from both the BEGA and parametric studies.

The EEGA was then applied towards the estimation of thermal properties. Here, the algorithm was used to minimize an objective function based on the least squares error. Two case studies involving nonlinear parameter estimation were used to demonstrate the effectiveness of the EEGA. The first concerned the simultaneous estimation of two and three thermal properties of an anisotropic composite material using the experimental designs optimized in the optimization test problems described above. These estimation problems were investigated previously by Hanak (1995). The second test case involved a one-dimensional transient analysis of combined conduction and radiation heat transfer in an insulative foam material (polystyrene) for the simultaneous estimation of four thermal and radiative properties. These included the effective thermal conductivity, volumetric heat capacity and extinction coefficient of the material, and the volumetric heat capacity of the heater. This study was realized in cooperation with J. Guynn (1996) as part of his master's thesis in Mechanical Engineering at VT. The results are not reported in this dissertation however, but can be found in the literature (Garcia et al., 1998). In both case studies, the properties were estimated as constants at ambient temperature.

Once the GA-based optimization/estimation methodologies were assessed, a study was conducted to evaluate the effects of the optimality criterion used for the experimental design on the accuracy of the estimated thermal properties. The one- and two-dimensional transient heat transfer analyses associated with the simultaneous estimation of two and three thermal properties of an anisotropic material (Hanak, 1995) and discussed previously, were also used here. The experimental designs in both analyses were optimized using the *A*-, *D*-, and *E*-optimality criteria, which are the three main criteria proposed for the design of experiments. Based on these optimal designs, simulated data were generated using an analytical mathematical model of the design. The thermal properties were then estimated from the simulated data from each experimental design, and the confidence intervals of the resulting estimates were compared. EEGA was used as both the optimization and estimation methodologies.

The completion of the first three specific objectives concluded the first stage of this dual Ph.D. program initiated at VT. The genetic-based optimization and estimation methodologies developed at VT were used by Hanuska (1998; also in Hanuska et al., 1999) for the thermal characterization of a complex aerospace structure (composite/honeycomb panel). This work was performed as part of his master's thesis in Mechanical Engineering at VT and concluded the multi-year research cooperation sponsored by the Thermal Structure Branch of NASA Langley Research Center.

The second stage of this dual program was performed at the LTI in Nantes. Efforts focused on accomplishing the last two specific objectives. Prior to formulating a general-purpose computer program, a third GA, GA_3, was developed built upon both the previous work and the experience gained in the GA field. The algorithm was then constructed in two parts, an invariant and an adaptation part, following the structure of the program CONDUCT developed by Patankar (1991). The invariant part contains the general calculation scheme that is common to all possible EDO/SPE problems within the overall restrictions of the program. It is written without any knowledge or assumption about the particular details of the problem to be solved. The user provides the problem specification in the adaptation part. Based on the GA_3 structure, two versions were developed. The GAMAIN version was designed for the analysis of any optimization/estimation problems for which a mathematical model can be provided in the adapt part. In heat transfer analyses for which an analytical solution cannot be obtained, the GACONDUCT version was used. The latter combines the feature of GA_3 with

a finite difference program based on an extension of the program CONDUCT. Therefore, the use of GACONDUCT allows for any EDO/SPE applications that deal with the computation of conduction and duct flow heat transfer in two-dimensional rectangular or cylindrical geometry.

To illustrate the performance of the GA_3, a mathematical function called f6 (Davis, 1991) was optimized using GAMAIN. This test case was also used as a basis for the investigation of the effects of some genetic operator variants in terms of convergence of the algorithm.

The general-purpose optimization/estimation GA_3 program was then applied to a variety of EDO and SPE problems. The applications performed were in agreement with the research environment at the LTI. As part of an industrial contract, the GACONDUCT was used in the simultaneous estimation of the thermal properties of composite materials (effective thermal conductivities perpendicular and parallel to the fibers and volumetric heat capacity) over the temperature range [30-150°C]. To take into account the temperature dependence in the properties, these latter were sought to be estimated as constant at six different temperature levels that covered the required range. Taking advantage of the estimation problem similarities with the two-dimensional transient heat transfer analysis performed by Hanak (1995), experiments were based on the same basic experimental design, and the same nondimensional optimal experimental parameters were used. Additionally, this study required the use of an apparatus to control the initial temperature inside the samples. An interesting personal aspect of this application was the opportunity to gain experience in conducting experimental work. This study was then used as a basis to investigate the optimization of the experimental design for the simultaneous estimation of parameters describing the temperature dependence in the thermal properties. This dependence was approximated by a piece-wise linear function with temperature. Nine parameters were used to represent the thermal properties over the range [25-150°C]. The *D*-optimality criterion was used to optimize seven experimental parameters. These latter included sensor location, heating parameters, and heating area. The estimation methodology was then demonstrated on simulated data generated from the optimal design.

The GACONDUCT was also applied to the simultaneous estimation of seven thermophysical parameters associated with the processing of composite materials in a two-dimensional RTM (Resin Transfer Molding) mold. This work was performed in cooperation with D. Lecointe (1999) as part of his PhD project at the LTI. The parameters estimated

included the temperature dependence of the material thermal properties over the range [100-130°C]. The results obtained were compared with those from Lecointe who used a parametric study to estimate the conductivity parallel to the fibers assuming both the orthogonal component and the volumetric capacity to be known.

Finally, a study was conducted for the kinetic characterization of the curing of composite matrix materials, namely thermosetting materials. Such characterization is an important aspect in the control of the thermal phenomena during composite material fabrication. This control involves modeling the coupling between heat transfer and exothermic chemical reaction inside the matrix material and thus requires knowledge of the dependence with temperature of not only the thermal properties but also the rate of cure. This latter is described by a kinetic model governing the curing process. Because of its popularity in the composite industrial world, the model from Kamal and Sourour (1973) was selected for the prediction of the curing process of an epoxy, a polyester and a rubber. Furthermore, the use of this model provided the investigation of a complex simultaneous estimation problem as strong correlations are present among the kinetic parameters involved. The general-purpose program GAMAIN was applied for the determination of these parameters. The experimental data required in the estimation methodology were obtained from Differential Scanning Calorimetry (DSC).

CHAPTER 2

Literature Review

This chapter summarizes the present state of knowledge pertaining to the areas of interest of this research. These are thermophysical characterization of composite materials, experimental design optimization, and Genetic Algorithms (GAs). After a brief description of composite materials in the first section, the second deals with both thermal characterization of composite materials and kinetic characterization of the curing of composite matrix resins. Particular attention is given to optimal experiments designed for the estimation of thermal properties in the third section, while the review of previous uses of GAs in the last section focuses on their application in engineering.

2.1 Composite Materials

A composite material is composed of two or more materials joined together to form a new medium with properties superior to those of its individual components. Often, the term composite is used for fiber-reinforced composites, although different reinforcement forms exist. Fiber-reinforced composites (laminates) consist of several unidirectional layers arranged at the same or different angles and, therefore, present heterogeneous, anisotropic properties. These materials can be classified as continuous or discontinuous. The most commonly used reinforced fibers are carbon/graphite and glass, while the major types of matrix resins consist of thermosetting, elastomer and thermoplastic materials with the addition of a curing agent. The composite materials and matrix resins focused on in this study consist of continuous carbon fiber/epoxy matrix combinations (with unidirectional fibers), and epoxy, polyester and rubber mixtures, respectively.

The use of composite materials is constantly increasing in modern industry. The main

reasons are low weight, high performance in terms of both mechanical and thermal properties, and relatively low cost. The study of the different aspects of physical and chemical phenomena taking place during material production is therefore of intensifying interest. In order to predict and control the fabrication/molding processes, thermophysical characterization of these materials is required. Due to the high coupling between heat transfer from conduction within the composite being cured and heat release from exothermal effects of the reticulation reaction, such characterization is comprised of both thermal and kinetic components. This necessitates that the thermal properties and the parameters of the kinetic model governing the curing process are known.

On one hand, because a composite is made of at least two different materials each with different thermal properties, effective thermal properties are usually needed and were considered in this research, assuming the materials to be homogeneous in each direction. Therefore, in the work presented here, the subscript “eff” was omitted. The thermal properties estimated were the thermal conductivity and volumetric heat capacity. These properties depend on temperature and as a result of fiber orientation, the thermal conductivity is also directionally dependent. Both temperature and directional dependence make the determination of the thermal properties a challenging task.

On the other hand, the kinetic parameters to be determined are associated with the model selected to govern the curing of the matrix resin. Therefore, one difficulty in adequate kinetic characterization is the selection of an appropriate model.

2.2 Thermophysical Characterization of Composite Materials

2.2.1 Thermal Characterization

Much work has been done for the accurate determination of the thermal properties of isotropic and anisotropic materials. Parameter estimation techniques can be typically classified as experimental and inverse. Experimental techniques are associated with a particular experiment (the technique is actually referred to by the name of the experiment), while inverse techniques include a wide variety of methods, all of which involve the use of experimental data in conjunction with a mathematical model describing the thermal phenomena. In the field of composite materials, a third class of techniques exists, which is

commonly referred to as analytical (also called “micromechanical”). The following provides a synopsis of the three classes.

- **Analytical methods**

Analytical methods are based on the mathematical analysis of the components of the composite. Their use involves the assumption that the thermal properties of the individual composite elements, namely the matrix and the fiber, are known, along with the volume fraction of the fibers. Several such models for the effective thermal properties of composites have been proposed. One very well known model is the Rule-of-Mixtures for which one can write

$$k = k_f V_f + \left(1 - V_f\right) k_m \quad \text{and} \quad \frac{k}{\rho C_p} = \frac{V_f k_f + V_m k_m}{V_f \left(\rho C_p\right)_f + V_m \left(\rho C_p\right)_m} \tag{2.1}$$

where k is the thermal conductivity with heat flow parallel to the fibers, (ρC_p) is the volumetric heat capacity, k_f and $(\rho C_p)_f$ and k_m and $(\rho C_p)_m$ are the properties of the fiber and the matrix, respectively, and V_f and V_m are the fiber and matrix volume fraction, respectively. Progeholf et al. (1976) indicated that none of the correlations developed accurately predicts the thermal properties of all types of composites. Their work also provides a review of additional models to predict the thermal conductivity of composite systems.

- **Experimental Methods**

Experimental methods can be further classified into steady-state and transient methods (Degiovanni, 1994). Steady-state techniques are limited to the sole estimation of thermal conductivity. The guarded hotplate method is a frequently used steady-state technique in which the specimen is heated by a hot metal plate attached to it and the resulting temperature is measured at the interface. The (effective) thermal conductivity is directly determined from Fourier’s law. One disadvantage with this technique is that it is expensive and time consuming due to the necessity for the experiment to be repeated at different temperature levels, and for the material to reach steady state.

Transient techniques allow for the estimation of several properties, such as the thermal diffusivity, thermal conductivity and/or other groups incorporating the conductivity and volumetric heat capacity. The most common transient method is the flash method in which the front surface of a small cylindrical specimen is exposed to an energy pulse and the temperature history is recorded on the back surface. The thermal diffusivity is identified from adjusting the theoretical temperature history obtained from a mathematical model to the measured temperature history. This can be achieved from the use of two different estimation methodologies (André and Maillet, 1999):

1/ the solution from analytical expressions associated with the knowledge of the Fourier number from either two partial times or two periods.

2/ the minimization of the least-squares error between calculated and measured data over several observations. The definition of this error as well as the inverse estimation procedure needed to minimize it are discussed later. Researchers at the Laboratoire d'Energétique et de Mécanique Théorique et Appliquée (LEMTA, Nancy, France), for instance, use successively both estimation methods (André and Maillet, 1999).

The heat capacity is typically determined using Differential Scanning Calorimetry (DSC). This experimental method is based on the principal of differential enthalpic analysis and involves providing heat both to a very small sample and to an inert reference sample at a varying rate so as to maintain their temperatures equal. The calorimeter is employed in scanning mode to determine the heat capacity as function of temperature. The product of the heat capacity with density results in the volumetric heat capacity.

The guarded hotplate, the flash, and the DSC methods are the major experimental techniques currently used to determine the thermal properties of composite materials. One however realizes that these methods do not allow for either the simultaneous estimation of the thermal properties, or the investigation of complex structures involving several materials which cannot be disassembled. In addition, besides the DSC method, the other methods are limited to the estimation of constant properties at a particular temperature level.

- **Inverse Methods**

Definition

The limitations of the experimental methods have led to the increased use of inverse parameter estimation techniques. Note that in the heat transfer area, one commonly refers to parameter estimation problems as the problems of determining unknown thermal properties based on known boundary and initial conditions, while inverse heat conduction problems are associated with the finding of boundary and initial conditions (function estimation) given known thermal properties. Parameter estimation methods are non-invasive techniques that allow for the simultaneous estimation of the thermal properties of individual materials as well as complex structures for any kind of appropriate experiments, provided these are feasible and a mathematical model can be formulated. “Appropriate experiments” implies that information is provided about the unknown properties. For instance, it is necessary for the experiments to be transient to estimate the volumetric heat capacity and for one of the boundary conditions to be a heat flux condition in order to estimate thermal conductivity and volumetric heat capacity simultaneously.

Inverse parameter estimation methods are based on the minimization of an objective function containing both calculated and measured temperatures (Beck and Arnold, 1977). Depending on the amount of information available about the experimental data and the parameters to be estimated, three main estimators are available to define the objective function. These include:

1/ Ordinary Least Squares (OLS) estimator, in which no prior knowledge about either the parameters estimated or the variances of the measurement errors is required.
2/ Maximum Likelihood (ML) estimator, in which prior knowledge about the variance of the measurement errors can be implemented.
3/ Maximum A Posteriori (MAP) estimator, in which prior knowledge about the variance of both the measurement errors and the estimated parameters is used.

All three estimators are described in detail by Beck and Arnold (1977). The OLS estimator is by far the most frequently used for the estimation of thermal properties as no prior knowledge is needed. This estimator was considered in this research. The associated objective function, the least squares error S, is expressed by:

$$S(\beta) = \sum_{k=1}^{N_k} \sum_{i=1}^{N_i} \left[T_{ki}(\beta, \tilde{x}, \tilde{t}) - \tilde{T}_{ki} \right]^2 \qquad (2.2)$$

where $\boldsymbol{\beta}$ is the true parameter vector containing the unknown thermal properties, $\tilde{x}$ and $\tilde{t}$ are position and time for the i^{th} observation from the k^{th} sensor, N_k and N_i are the numbers of sensors and observations, respectively, T is the calculated temperature from the mathematical model governing the heat transfer phenomena and $\tilde{T}$ is the measured temperature. In using Eq. (2.2), the thermal properties are found by minimizing the sum of squared differences between the measured and calculated data. It should be mentioned that if the parameters are to be estimated from measurements of two dependent variables, say T and q, then the least squares errors associated with each dependent variable should be nondimensionalized by dividing by the respective measurement variance, allowing thus the addition of both errors to form a global error. This was investigated by Robinson (1998). Note also that although parameter and function estimation problems are both inverse problems, the ill-posedness of the latter may require the addition of regularization terms in the objective function (Beck et al., 1985).

Techniques

The minimization of Eq. (2.2) could conceivably be performed by any optimization technique. However, parameter estimation has generally been performed with only a few methods, none of them being a standard. Actually, the use of one method over another is often specific to a certain field of study. The simplest parameter estimation method is the parametric study, which is a numerical iterative method. This study is usually performed in two phases: the first includes determining the general range of the properties optimal values, while the second narrows this range to determine the values more precisely. If needed, the process is repeated to converge to the final estimates. As one can easily guess, this technique is tedious and time intensive and, in addition, the process does not guarantee that the global minimum of S will be found. But, because it is so easy to implement, the parametric study is often used to estimate one or two properties.

One commonly used gradient-based technique is the Gauss linearization method which is a first unconstrained descent method. The minimization of S is realized by differentiating S with respect to $\boldsymbol{\beta}$, setting the resulting equation equal to zero, and then solving iteratively for $\mathbf{b}$, the estimated parameter vector for $\boldsymbol{\beta}$ using the Taylor series approach to linearize the

equation. This method is described (Beck and Arnold, 1977) as one of the simplest and most effective methods for seeking minima provided the initial estimates are in the neighborhood of the minima, and this latter is reasonably well defined. In this last condition it is meant that, on one hand, the dependent variable (usually T) is sufficiently sensitive to changes in the properties, and on the other hand, the properties are far from being nearly correlated. Box and Kanemasu (1972) modified the Gauss method by changing the step size used in seeking minima with an aim to compensate for poor initial estimates or severe nonlinearity in the model which could cause large oscillations to occur from one iteration to another, leading then to non-convergence of the estimates. A further improvement involving the check that the function S decreased from one iteration to another was realized by Bard (1974). This consisted in reducing the step size by one-half if the function was not decreasing. The modified Box-Kanemasu method, however, still required the minima to be reasonably well-defined as explained above. Theoretical details on this method are given in Chapter 3.

Beck was the first to use the Gauss method to estimate the thermal diffusivity in 1963. He then expanded the Gauss application to the estimation of the thermal conductivity simultaneously with the volumetric heat capacity of nickel from one-dimensional transient temperature measurements (1966). The simultaneous estimation of the thermal conductivity perpendicular to the fiber plane and the volumetric heat capacity of composite materials has been widely performed using both the Gauss and modified Box-Kanemasu methods. Scott and Beck (1992a) estimated these thermal properties for carbon/epoxy composites as function of temperature and fiber orientation. Their results show that the thermal properties increase with temperature and that different stacking orientations result in significantly different thermal conductivity values. These authors also developed a methodology for the estimation of these two properties in the same composite materials during curing (1992b). Garnier et al. (1992) were able to estimate these two properties using temperature measurements made with thin resistance thermometers and surface thermocouples instead of internal temperature measurements. The work from Moncman (1994) and Hanak (1995) show that the simultaneous estimation of the thermal conductivity perpendicular to the fiber plane and the volumetric heat capacity of composite materials has become successfully routine. The Gauss method was also used by Jurkowski et al. (1992) for the simultaneous estimation of the thermal conductivity of thermoplastic materials and thermal contact resistance, assuming the volumetric heat capacity to be known. As in the work from Garnier et al. (1992), no embedded sensors were used. One interesting conclusion from this study is that small

sensitivity coefficients or the unbalance of the sensitivity matrix resulted in the instability of the estimation procedure. This particular remark goes along with the fact that both the Gauss and modified Box-Kanemasu methods have been found to show instabilities resulting in non-convergence when used with models that contain correlated or nearly correlated thermal properties. For instance, Hanak (1995) used the modified Box-Kanemasu method in association with two-dimensional transient experimental data and was unable to simultaneously estimate the thermal conductivities along two perpendicular planes and the volumetric heat capacity of anisotropic composite materials because of correlation between both thermal conductivities. Copenhaver (1996; also in Copenhaver et al., 1998) was also faced with non-convergence of the modified Box-Kanemasu method when trying to simultaneously estimate correlated radiative and conductive properties of a honeycomb sandwich structure. A quantification of correlation is given in the next chapter (Section 3.1.3).

Several different approaches have been used to address this correlation-based non-convergence problem. One approach is to modify the experimental design. For example, Loh and Beck (1991) were able to simultaneously estimate both thermal conductivities and the volumetric heat capacity of an anisotropic carbon/epoxy composite through the use of nine thermocouples embedded at various locations within the sample. It is interesting to note that the number and location of the sensors were fixed a priori by the authors and the potential correlation problem was never detected. Correlation may have still been present but the use of multiple sensors allowed it to be bypassed. Box has actually shown that high correlations among the parameters can be due to a large extent to the nature of the model itself and thus no experimental design could be expected to yield uncorrelated parameter estimates (Beck and Arnold, 1977). Loh and Beck used the Gauss method and found the conductivity parallel to the fiber plane to be about seven times larger and to increase more with temperature than tranverse to the fiber plane. A similar approach was accomplished by Dowding et al. (1996) for the simultaneous estimation of the thermal properties of anisotropic carbon/carbon composites. Nevertheless, modifications of the experimental design, such as the use of internal sensors, are not always feasible, especially when nondestructive testing is required. In addition, the use of embedded thermocouples can be a source of important bias. In characterizing this bias, Taktak (1991) reported that experiments showed higher dependence of the temperature disturbance on errors in the embedded thermocouple locations than errors in the thermal properties. Another approach used to address the correlation problem is to modify the minimization method. For example, Copenhaver (1996) (note also Copenhaver et

al., 1998) used a constrained parameter estimation procedure based on a penalty function method, with limited success, to simultaneously estimate three nearly correlated thermal properties of a honeycomb sandwich structure.

The approach investigated in the present work involves the use of a robust non-gradient method, namely the Genetic Algorithm (GA) method, in the minimization procedure. The motivation for using GAs was to circumvent difficulties of non-convergence in cases when the parameters are correlated or nearly so. An overview of these algorithms is provided in the last section of this chapter.

2.2.2 Kinetic Characterization

The curing of thermosetting materials is a complicated process, the main parts of which are chemical transformation coupled with heat transfer. For the chemical transformation and more particularly, the exothermic source term, to be characterized, a kinetic model is required. Kinetic models can be divided into two general types: on one hand, the models based on the knowledge of each elementary chemical reaction, and on the other hand, the empirical ones that try to represent the kinetics of reactions when the reaction path is not well known. These latter have the advantage of allowing for the analysis of complex transformations, which is the case for the curing of elastomer or thermosetting compounds used in molding processes. They provide relationships between reaction rate ($d\alpha/dt$), degree of reaction (α) and temperature (T). In the field of thermosetting polymers, several different empirical models have been developed to characterize curing. They are often referred to as describing autocatalyzed reaction rate mechanisms as the material contain substances (curing agents) that accelerate the reaction rate. Figure 2.1 illustrates a typical reaction rate evolution versus time during curing of a thermosetting material. For the complete representation, the kinetic model is preceded

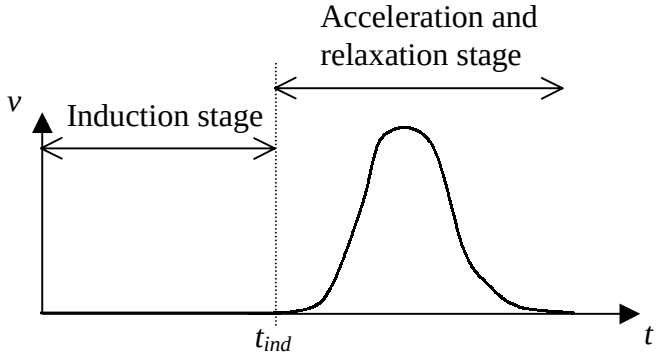

Figure 2.1 Typical reaction rate evolution versus time during curing of thermosetting polymers.

with a model describing the induction stage, t_{ind}. This represents the time during which the reaction is inhibited as a result of inhibition substances contained within the material.

The model from Kamal and Sourour (1973) is a very well known empirical kinetic model, which has been found to provide a reasonable degree of accuracy for a variety of thermosetting systems. It contains two rate constants K_1 and K_2 that are assumed to have an Arrhenius temperature dependence and two kinetic exponents *m* and *n* to describe the order of the curing mechanism as shown below.

$$\frac{d\alpha}{dt} = \left(K_1 + K_2 \times \alpha^m\right)(1-\alpha)^n, \quad K_i = A_i \exp\left[-\frac{E_i}{RT}\right], \quad i = 1,2 \tag{2.3}$$

The parameters K_1 and K_2 represent the catalytic and the autocatalytic nature of the reaction, respectively. When the parameter K_1 is negligible, the terms containing the dependent variables *T* and α can be mathematically separated. The model becomes then similar to that suggested by Piloyan et al. (1966). Jarny et al. (1993) developed for that case a new model expressed by the product of a rate constant *K* that follows the Arrhenius law and a polynomial function of α expressed below:

$$\frac{d\alpha}{dt} = K(T) \times F(\alpha) \tag{2.4}$$

The model from Jarny et al. has been successfully applied to the kinetic characterization of the curing of a rubber (Amiaud, 1993), an epoxy (Bailleul, 1993; 1997; Bailleul et al., 1996), and a polyester resin (Mouchnino, 1997).

Using the kinetic model from Kamal and Sourour (1973), one typically assumes a known combined order mechanism (*m*+*n*), which is generally second order (Kamal et al., 1973), and therefore the parameters estimated are the two rate constants K_1 and K_2. The most commonly used method of determining them involves the use of linear regression and isothermal Differential Scanning Calorimetry (DSC) which provides heat flux measurements. The rate constants are identified at different temperatures from which the Arrhenius constants can be deduced. One of the disadvantages with this approach is that the Arrhenius constants cannot be estimated directly.

An alternate approach is to use an inverse parameter estimation method that can be used for nonlinear models. As mentioned in the previous section, this involves the minimization of an objective function, for instance the least squares error. Scott and Saad (1993a,b) studied the model from Kamal and Sourour assuming a combined second-order, autocatalyzed reaction

rate mechanism during the first portion of the cure to describe the curing of an amine epoxy resin. Using the Box-Kanemasu method, they were able to perform the direct estimation of the four Arrhenius constants from both isothermal DSC and dielectric data. They conducted sensitivity analyses that showed that the degree of cure was most sensible to changes in the parameters K_1 and K_2 than the rate of cure. Furthermore, Scott and Saad pointed out that the use of the degree of cure as the dependent variable associated with isothermal data allowed minimization of the correlation between the sensitivity coefficients of the parameters and maximization of their magnitudes. On the contrary, strong linear dependence between the coefficients of the parameters A_1 and E_1 and A_2 and E_2 was stressed when using dynamic data. In comparison with the commonly used linear regression method, the work by Scott and Saad is a great improvement in the curing characterization of epoxy systems. However, their study assumed a known combined order mechanism, restricting thus the estimation procedure to the four Arrhenius parameters. In addition, by limiting the estimation procedure proposed by Scott and Saad to isothermal experiments, one cannot investigate materials that react very fast and for which only dynamic data can be obtained.

For the cure modeling of a polyester resin, Guyonvarch (1995; also in Guyonvarch et al., 1995) also used the model from Kamal and Sourour in association with isothermal DSC data. To limit both the number of parameters to be estimated and the presence of correlation among the sensitivity coefficients, he assumed the parameter m to be known, and set its value arbitrarily to unity. His work involved the application of the Gauss-Newton method in two steps: first, he tried to identify simultaneously the rate constants K_1 and K_2 along with the parameter n; next, he fixed n to the average estimated value obtained previously (with an error of ± 18 %), and determined the values of K_1 and K_2. Eventually, knowing K_1 and K_2 at each different temperature investigated, the four Arrhenius constants could be found from a graphical procedure. It is interesting to note that simulations using the completed kinetic model fit isothermal DSC runs well, but were relatively far off when dynamic DSC data were considered.

One can note the work of Bournez et al. (1999) who investigated the estimation of five kinetic parameters associated with an equation derived from the Kamal and Sourour model, simultaneously with the thermal properties (conductivity, heat capacity and density) of a rubber modified epoxy resin. Their work presents a methodology to determine these thermophysical parameters from a single dynamic experiment carried out in an experimental mold. The Gauss method and the MAP estimator were used as the estimation procedure.

However, because of significant magnitude differences between the sensitivity coefficients of the parameters, the simultaneous estimation was restricted to a sequential estimation by groups of parameters of similar influence (sensitivity) on the temperature response. The most influential parameter was found to be the Arrhenius constant *E* of the kinetic model used, and was identified alone first.

The limitations of the work of Scott and Saad (1993a,b), Guyonvarch (1995) and Bournez et al. (1999) show that the investigation of nonlinear kinetic models, and in particular the model from Kamal and Sourour, in association with the use of dynamic experimental data remains a very difficult estimation problem. The difficulties come mainly because of strong correlations and difference of influence (sensitivity) on the model among the parameters. The ability to solve such estimation problems would be particularly significant in the field of composite matrix resins as kinetic models are used to characterize curing during fabrication processes which involve dynamic experiments. This was one of the objectives of the work presented here.

It is relevant to note that with the use of the two kinetic models described in Eqs. 2.3 and 2.4, an induction period should be defined to represent the time during which the reaction is inhibited, e.g., corresponding to null thermal effects, as illustrated in Fig. 2.1 (Garnier, 1990). This period is governed by its own kinetic model that depends both on temperature and on the "thermal history" of the material being analyzed. Bailleul (1997; also in Bailleul et al., 1996) used an integral function $h(t,T)$ that is a function of time and which represents (in absolute value) the time left before curing starts. The induction period, t_{ind}, is over when the function $h(t,T)$ becomes null.

$$h(t,T) = t_{ref} - \int_0^t \exp\left[- B \times \left(\frac{T_{ref}}{T} - 1 \right) \right] dt \qquad (2.5)$$

The inhibition model described by the function $h(t,T)$ involves the selection of an arbitrary reference temperature, T_{ref}, within the range investigated and the determination of two parameters, t_{ref} and B. This estimation is very difficult because of the correlation between the sensitivity coefficients of the two parameters, and typically the values for t_{ref} and B are obtained using a parametric study. The inhibition time model used in the current research for the kinetic characterization of the curing of thermosetting materials (Chapter 6) is based on a modification of Bailleuil's integral function.

Eventually, to obtain the experimental data required in the estimation procedure, calorimeters such as Differential Scanning Calorimetry (DSC) apparatuses are usually used because heat flux released by the chemical reaction is proportional to the rate of reaction (Scott and Saad, 1993a,b, Garnier et al., 1993). As far as the evaluation of DSC apparatus is concerned, three precision indicators have been proposed by Garnier and Danès (1994). These indicators are based on isothermal operation of the DSC while empty, and include a time constant from a constant slope increase to a constant level, a time drift and background noise. Note however, that some recent work (Sommier, 1998) has shown for some thermosetting materials the feasibility of using microdielectrometry for the online study of degree of cure evolution during curing.

2.3 Experimental Design Optimization

This section deals with optimization in the service of design-of-experiments, that is optimization employed to provide the maximum amount of insight and information on the phenomena being analyzed. A review of optimization in relationship to experiments in four aspects has been reported by Haftka et al. (1997). These aspects include the use of optimization for designing efficient experiments (called “analytical optimization”, the subject of this section), the use of experiments to perform optimization (called “experimental optimization”), the use of techniques developed for experimental optimization in numerical optimization and eventually, the importance of experimental validation of optimization. In their review, Haftka et al. provide applications from a variety of fields.

Design-of-experiments for the estimation of parameters has been subject to numerous studies. Most of the early publications deal with the field of statistical inference and data analysis (Brown et al., 1985), while an increasing number of publications can be found over the past two decades in the field of engineering design. When the purpose of the experiments is to estimate properties, the objective of experimental design optimization is to improve the accuracy of the predicted properties. The selected design variables are “sized” to minimize the uncertainty in the resulting property estimates, thus providing the most accurate estimates (Beck and Arnold, 1977; Walter and Pronzato, 1994). Design-of-experiments can be performed simply by carefully examining the sensitivity coefficients of the parameters to be estimated or, in a more rigorous methodology associated with optimal experimental design theory, by applying an optimality criterion. In both cases, this procedure is an imperative step prior to the implementation of the inverse parameter estimation procedure. Based on the book

of Beck and Arnold (1977), the work of Raynaud (1999) illustrates with simple examples the various steps that must be accomplished in the strategy for optimization of experimental design and estimation of parameters.

2.3.1 Sensitivity Study

First of all, a careful sensitivity study can enable the distinction of which properties can be correctly estimated (known as identifiability study). The sensitivity coefficients are the derivatives of the experimental process variables, such as temperature, with respect to the unknown parameters, for example, the thermal conductivity. Obviously, uncorrelated parameters with the highest sensitivity coefficients should be chosen to be identified. In the analysis of sublimation-dehydration within a porous medium, Scott (1994) conducted a sensitivity study which examined the importance of the material properties on the solution. Scott was able to conclude for which parameter temperature provided the most accurate information. A similar study was performed by the current author (1994) in investigating the simultaneous estimation of the thermal conductivities of individual components constituting high temperature superconductive thermal bridges. She found that only the effective thermal conductivity of the composite superconductive thermal bridges could be estimated.

Sensitivity studies also allow improvement of an experimental design to be used in the determination of properties by selecting experimental conditions that minimize sensitivity to parameters assumed known (set to nominal values) in the mathematical model. This ensures that uncertainty from these supposedly known parameters does not greatly affect the accuracy of the estimation of the unknown desired parameters. One example in which such a sensitivity study is particularly adequate is in the investigation of the effect of convection heat transfer coefficients used at boundary conditions. Usually, the sensitivity to these parameters is low at the beginning of the experiments and then increases. The choice of the optimal total overall experimental time should take into account that the sensitivity to the known convection heat transfer coefficients must remain low.

Sensitivity studies can also be used to find the experimental conditions that maximize the magnitude of the sensitivity coefficients of the unknown parameters. However, one can easily guess that when two or more parameters are sought, the use of the magnitude of the individual sensitivity coefficients as a reference becomes messy and, therefore, the design activity needs to be posed in terms of an optimality criterion (objective function) to maximize. The work of Totorelli and Michaleris (1994) that reviews the state of design sensitivity

analysis is noted. This review shows that sensitivity applications in optimization are numerous and gives many references, including those for thermal systems.

2.3.2 Optimality Criterion

- **Definition**

An optimality criterion can be interpreted as a measure of the goodness of the design. Although its establishment should not be codified in terms of a single recipe, the optimality criterion is usually associated with the Fisher information matrix of the design (named after R. A. Fisher's pioneering contributions to statistical inference, Kiefer, 1975a; Walter and Pronzato, 1994). The Fisher information matrix is defined by $\mathbf{X}^T\mathbf{X}$, where $\mathbf{X}$ is the sensitivity matrix. The most often encountered optimality criteria include the maximization of the determinant of $\mathbf{X}^T\mathbf{X}$ (*D*-optimality), maximization of the minimum eigenvalue of $\mathbf{X}^T\mathbf{X}$ (*E*-optimality) and maximization of the trace of $\mathbf{X}^T\mathbf{X}$ (*A*-optimality). Theoretical details on these criteria are given in Chapter 3. The first criterion is the most common. Note that Alifanov et al. (1995) have shown that an optimality criterion based on the maximization of the inverse of the condition number of the Fisher information matrix is the most appropriate for the study of heat conduction, but that the use of *D*-optimality is nearly equivalent. The effect of *D*-optimality is, in the normal case, to minimize the volume of the usual confidence ellipsoids of the estimated values, providing the minimum variance estimators. *D*-optimality proponents have also pointed out that this criterion is invariant under linear transformation of the estimated vector. That is, the same design is *D*-optimum for estimating $Z\beta$ as for estimating β if Z is a nonsingular matrix. However, this criterion has been found to weigh heavily on the parameters with the highest sensitivity while sacrificing much in the accuracy of the parameters with the least sensitivity in order to make the confidence volume small (Kiefer, 1975b; 1981). For instance, in the design of experiments for the thermal characterization of honeycomb core structures (conductive and radiative properties), Copenhaver (1996) pointed out that the use of the *D*-optimality criterion would increase the accuracy of the parameters with high sensitivity at the expense of creating a large error in those with low sensitivity. Other known criteria associated with the Fisher information matrix exist, for instance the *C*-, *L*-, *V*- and *G*-optimality, with the latter two being more appropriate for response estimation than parameter estimation. This family of criteria has been discussed in more details by Kiefer (1974; 1975a) and Walter and Pronzato (1990).

Another strategy in the selection of the objective function is to develop a compromise or compound criterion (Kiefer, 1974; 1975b). This heading describes criteria "built-up" from simpler criteria. Such a strategy has the effect of combining the features and/or of eliminating some of the objections of the single criteria used to build up the compound criterion. Pronzato and Walter (1989) defined the *V*-criterion, which is similar to the *D*-optimality criterion, but which assumes that prior lower and upper bounds are available for the noise associated with the measurements. Because of the shortcomings displayed by the *D*-optimality criterion, Copenhaver (1996) used a combination of *D*-optimality with the minimization of the maximum scaled length of the confidence intervals. This latter criterion was actually proposed earlier by Lohman et al. (1992). The work from Nenarokomov et al. (1998) is a recent example of the use of a compound criterion, in which not only measurement noise but also uncertainties in the known model parameters have been incorporated in the *D*-criterion. Some previous developments have also emphasized the use of multicriteria optimization as a strategy in the design process (Eschenauer et al., 1990). This results from the fact that nowadays, in many engineering applications, often several conflicting criteria have to be considered by the designer. Such optimization problems for multiple criteria are called either *Vector* or *Multicriteria* Optimization Problems and the output from the optimization process is called a set of Pareto optimum. The utilization of multicriteria in the optimization of experimental designs used to estimate thermal properties has not been thoroughly investigated yet.

- **Optimization Techniques for the Design-of-Experiments**

Following the selection of the optimality criterion, a mathematical optimization procedure is needed to determine the optimal experimental parameters which satisfy the selected criterion. In the general field of design-of-experiments for the estimation of parameters, three classes of procedures have been distinguished. The first class contains exhaustive search algorithms which generate and evaluate all possible designs. This is very time consuming. Welch (1982) developed a variant called "branch and bound" in which a binary tree of minimization problems is generated. Not all designs are generated and evaluated. By exploiting bounds on the minimization, only the branches which might contain the optimal design are created. Although such algorithms guarantee that the global optimal design will be found, the computing costs are still extremely high. The second class includes analytical procedures which consist of maximizing the objective function by differentiating it with respect to each of the design variables and then solving the resulting set of equations

simultaneously for the optimal values of the design variables. Due to the complexity of the equations involved, this method is rarely chosen. Finally, the third class has usually been concerned with the exchange algorithms, which are iterative combinatorial random optimization procedures. Mitchell (1974) developed an efficient such algorithm called DETMAX which has been extensively used for determining *D*-optimum designs in a variety of engineering applications (Eschenauer et al., 1990). DETMAX is based on the notion of sequence of excursions from an initial design, in which several points are added in one single step and subsequently the same number of points that result in the smallest increase in the determinant (*D*-optimality) are removed. This algorithm was found to generate high quality *D*-optimal designs at relatively low computing costs but did not ensure that the global optimum will be found. Note that the "simulated annealing" approach, introduced by Kirkpatrick et al. (1983), was thought by Mitchell to be a potential optimization procedure to be applied to exchange algorithms for deriving experimental designs. What is interesting with this last remark is that simulated annealing and genetic algorithms, which were used in this work, share some of their stochastic steps.

- **Design-of-Experiment Applications for the Estimation of Thermal Properties**

In the design-of-experiments for the estimation of thermal properties, a simple iterative numerical approach, the parametric study, which belongs to the class of "exhaustive" procedures, has typically been used for its simplicity (Beck and Arnold, 1977). As described in Section 2.2.1, this methodology can get very confusing and time consuming for even a very few design variables. In addition, if the increment size is too large, the maximum determinant can be missed. Nevertheless, the parametric study has been extensively used with the *D*-optimality criterion. This technique was applied by Beck (1966) to determine the optimal conditions for the simultaneous estimation of the thermal conductivity and specific heat, and to determine the optimum transient experiment for estimating the thermal contact conductance (Beck, 1969). Taktak et al. (1991) used this procedure to estimate the thermal properties of isotropic composite materials by optimizing the number of sensors, sensor placement, and the duration of an imposed heat flux. A similar approach was performed by Garnier (1996) but for an insulating material in a cylindrical geometrical form. Based on the work from Taktak et al., one-and two-dimensional *D*-optimal experimental designs have also been developed by Moncman (1994; also in Moncman et al., 1995) and Hanak (1995) using a parametric study for the simultaneous estimation of thermal properties of anisotropic composite materials.

These included both the in-plane and through-the-thickness thermal properties. The Moncman and Hanak studies were used as test cases in the current work. Note that Hanak emphasized that one of the disadvantages of performing a parametric study is the possibility of overlooking the global optimum. Indeed, in studying the same two-dimensional design optimization analysis that Moncman had performed previously, using smaller increments to segment the design space, he found a design that produced a larger determinant than the optimal design developed by Moncman.

Recently, Rigollet et al. (1998) used *D*-optimality to investigate the optimal temporal domain for the most accurate estimation of the thermal diffusivity and effusivity of chromium coatings on steel. They use a pulsed photothermal method to obtain the required experimental data for the property estimation. From the estimates obtained, they could deduce the conductivity and volumetric heat capacity of the chromium coatings. Confidence intervals for these latter properties were calculated from classical logarithmic derivatives and comprised of both confidence intervals associated with the diffusivity and effusivity estimates considering measurement errors only, and those of supposedly known parameters (chromium effusivity and thickness of the coatings). Rigollet et al. showed that the uncertainties in the supposedly known parameters had by far the greatest effect on the accuracy of the calculated thermal conductivity and volumetric heat capacity. This work points out that not only should one focus on optimizing some critical design variables for the most accurate estimation of the unknown properties, but also, when preparing and conducting the optimal experiments, one should take care to minimize the uncertainties in other experimental parameters that are supposed to be known, such as material thickness. Note that a review of the most important sources of errors that can introduce bias in the final estimates can be found in Jarny and Maillet (1999).

Discussion of the present state of knowledge should be concluded with the importance for the optimal designs to be verified. This ensures that the best possible estimates have been obtained and allows for the validation of not only the optimization procedure but also the mathematical model used to describe the process. Hanak (1995) demonstrated that the optimal design provided the most accurate combined thermal property estimates by testing the optimal design along with two non-optimal designs. The non-optimal experimental parameters were chosen so that they did not satisfy the *D*-optimal criterion used in the optimization technique. Hanak's results showed that an individual property might be estimated with greater accuracy at a non-optimal setting but the combination of properties reached a higher accuracy at the

optimal setting. Validation of optimization through experiments is particularly relevant when the system is based on an analytical model which is not valid in the entire design space (Haftka et al., 1997).

2.4 Genetic Algorithms (GAs)

2.4.1 Description

Genetic Algorithms were developed by Holland (1975). Although these algorithms emerged simultaneously with two other streams known as Evolution Strategies (ES) and Evolutionary Programming (EP), GAs are today the most widely known type of evolutionary algorithms (Back, 1994). Differing from conventional search techniques, the common feature of these algorithms is to simulate the search process of natural evolution and take advantage of the Darwinian survival-of-the fittest principle. In short, Evolutionary algorithms start with an arbitrarily initialized population of coded individuals, each of which represents a search point in the space of potential solution. The goodness of each individual is evaluated by a fitness function which is defined from the objective function of the optimization problem. Then, the population evolves toward increasingly better regions of the search space by means of both random and probabilistic (or deterministic in some algorithms) biological operations. The three main evolutionary algorithms (GAs, ES and EP) were developed independently from each other as each emphasized different biological operators as being most important to a successful evolution process. The basic operators used in GAs consist of selection (the selection of parents for breeding), crossover (the exchange of parental information to create children) and mutation (the changing of an individual). In addition, following the Darwinian theory, an elitism operator (the protection of best individuals) is found in more elaborated GAs. The fundamentals behind GAs are detailed in Chapter 4, along with the relevant characteristics that differentiate these algorithms from conventional optimization methods. Note however here that the ergodicity of the biological operators used in GAs makes them potentially effective at performing global search (in probability) (Gen and Cheng, 1997). Also, GAs have the attribute of a probabilistic evolutionary search (although it is most commonly referred to as a randomized search), and are neither bound to assumptions regarding continuity nor limited by required prerequisites. Citing Goldberg (1989), GAs are blind.

Note that some efforts have been directed towards building an analogy between the representational mechanisms of GAs and their biological counterparts, thus producing a *lingo* (Goldberg, 1989 and Mitchell, 1996). In this correspondence terminology, an individual is thought of as a *chromosome* (*chromosomal string*) and the *genotype* is composed of the collection of possible chromosomes. Each chromosome consists of *genes* which may take on some number of values called *alleles*. Each gene has a particular *locus*, its position in the chromosome. Eventually, the solution point encoded by the chromosome represents the phenotype. This terminology, generally used within the GA field (artificial intelligence), was not used in this dissertation.

The GA technique has been theoretically and empirically proven to provide robust searches in complex spaces. Much of the early work of GAs used a universal internal representation involving fixed-length binary chromosomes with binary genetic operators. Consequently, most of the theory developed (which could fill several volumes!) is based on binary coding. In developing the Fundamental Theorem of GAs, Holland (1975) focused on modeling ideal Simple GAs (SGAs) to better understand and predict GA behavior [this theorem, also called the S*chema Theorem*, states that short, low-order schemata (particular genes sequences) with above-average fitness receive exponentially increasing trials in subsequent generations]. Many properties in terms of the binary genetic operators effectiveness were concluded from this theorem. However, Mitchell (1996) pointed out that these properties give some limited insight into the GA behavior. Mitchell believes that a more useful approach to understanding and predicting GA behavior would be analogous to that of statistical mechanics in physics whose traditional goal is to describe the laws of physical systems in terms of macroscopic quantities, such as pressure and temperature, rather than in terms of the microscopic particles (molecules) making up the system. Such an approach will aim at laws of GA behavior described by more macroscopic statistics such as “mean fitness in the population” or “mean degree of symmetry in the chromosomes” rather than keeping track of the huge number of individual components in the system (e.g., the exact genetic composition of each population).

Regarding theoretical guidelines about which GA to apply, the real problems encountered by GAs usually compel tailoring the GA at hand as the use of different encoding and operator variants could provide different solutions (Davis, 1991; Michalewicz, 1996). One realizes that there are therefore no rigorous guidelines for predicting which variants and more particularly, which encoding, works the best. By addressing the binary/floating point

debate, the work by Field (1996) confirms that there is no best approach and that the best representation depends on the problem at hand. Davis (1991) also recommends a problem-oriented approach, in which domain knowledge should be incorporated into the GA as much as possible, and the GA should be hybridized with other local optimization methods that work well. The current author believes hybrid GAs to be the most effective solution to complex optimization.

As one can understand, there are many controversies in the GA community over the approaches used, revealing that GA theory is by no means a closed book (indeed, there are more open questions that solved ones). One final point worth mentioning about the GA theory is that many of today's algorithms show enormous differences to the original SGA.

2.4.2 Applications in Engineering

Although the evolution simulation implemented in GAs appears to be a crude simplification of biological reality, over three decades of applications have clearly demonstrated the robustness of the resulting non-gradient algorithms. GAs have been applied to all (and more) of the areas Holland (1975) had indicated: optimization in engineering and computer science, combinatorial optimization such as job-shop scheduling, automatic programming and machine learning, biotechnology, economics and social sciences, financial forecasting, art and music, game-playing, to name the most relevant. Because of the complexity and the abstraction associated with the traditional binary coding generally used to encode design variables, research on GAs has been slow to spread from computer science to engineering. Over the past few years, however, application to real-world problems has increased greatly as many researchers started to adapt the algorithm encoding to the most natural representation of the search space. The *Handbook of Genetic Algorithms* (Davis, 1991) is a striking evidence of the possible real world GA applications in industry. Some recent interesting demonstrations of the effectiveness of GAs with both integer and real-number coding in the fields of structural optimization, and more particularly composite structure optimization, parameter estimation and thermal sciences are outlined below. Note that GAs have not been utilized very much in heat transfer.

In structural optimization, Furuya and Haftka (1993) determined optimal actuator locations on large space structures using GAs with integer coding. They showed that the performance of the algorithms with integer coding was at least as good as or better than the performance with binary coding. Doyle (1995) illustrated GAs with real-number coding to

efficiently locate the size and location of a crack in a frame structure. The inverse problem of identifying the number, location and shape of holes to make in structural components with an aim to optimizing their weight has been investigated by Nakamura and Taomoto (1996) using successively a GA and the conjugate gradient method. The design was performed in two steps: first, the total number of holes and their initial location and shape were estimated using the GA; then, the optimal shape and location were identified by the gradient-based optimization method.

For composite laminate design and optimization, Soremekum (1997) modified a basic GA to include a second chromosome string so that composite laminates comprised of multiple materials could be studied with greater efficiency. Using this modified GA, Soremekum performed the minimization of both the cost and weight of a simply supported composite plate under different combinations of axial loading, and obtained a Pareto-optimal set of designs. Multi-objective optimization of laminated ceramic composites was also previously performed by Belegundu et al. (1994) using GAs. Exploiting the GA property of implicit parallelism for the design of composite laminate structures, McMahon (1998) developed a distributed GA with migration which was aimed to operate on a parallel processor. The migration algorithm was found to diminish the normalized cost and improve the reliability of a GA optimization run.

Using GAs as a parameter estimation technique, Carroll (1996a and b) could simultaneously estimate a set of unknown parameters that best matched a chemical laser model prediction with experimental data. Jones et al. (1996) used GAs to determine the optical properties and the particle size distribution function of propellant smoke from angular light-scattering measurements. A combination of the gradient-based Gauss method and a GA was applied by Wright (1996) to determine the specific acoustic admittance of the inlet and outlet ports of a combustion chamber. By exploiting the advantages of both techniques, Wright was able to arrive at accurate estimates of the acoustic boundary conditions for nearly any candidate system. A similar procedure was conducted by Autrique and Souza de Cursi (1997) who implemented a stochastic modification based on GAs into classical gradient-based methods for the control of the vulcanization process. They showed that such an implementation was efficient for global optimization. Raudensky et al. (1995) applied GAs in solution of inverse heat conduction problems, while a GA for an inverse radiation problem was used by Li and Yang (1997). Lorion et al. (1999) have just reported the use of GAs for the successful estimation of thermal diffusivity in a multi-layer material. Their work also involves a comparison of results obtained on a homogeneous material using both GAs and the

Levenberg-Marquard method. In this comparison, GAs were found to provide more accurate and stable results than the gradient-based method.

The feasibility of GAs to solving heat transfer problems was illustrated by Davalos and Rubinsky (1996). In this work, two simple cases of conduction heat transfer were considered. These included 1) conduction in a one-dimensional slab, with one side kept constant at the temperature of zero which was also the initial temperature, while the other side temperature changed with a constant rate; and 2) conduction in a two-dimensional square in which the temperature of three sides was zero (also the initial temperature), while the temperature on the fourth side changed with a constant rate. The temperature distribution was encoded as a string of normalized temperatures (the parameters to determine) at discrete spatial and temporal locations. The fitness function to evaluate the chromosomes was based on the conservation of energy incorporating both local and global conservation. For both test cases, the accuracy of the results obtained with the GA was remarkable.

In the field of thermosciences, the optimized cooling of electronic components is one intractable optimization problem type that requires the use of GAs. Queipo et al.(1994) used these algorithms to find optimal or nearly optimal arrangements of convectively cooled components placed in-line on the bottom wall of a ventilated two-dimensional channel. They concluded that GAs allow a cost effective approach for investigating highly complex numerical and experimental thermoscience problems where it is desirable to obtain a family of acceptable problem solutions, as opposed to a single optimum solution. This work showed the adaptability of GAs. In the optimization of a chip design layout on a circuit board, Sakait and Chang (1996) were also able to easily take heat source constraints into consideration using GAs. These algorithms were used as well for the thermal design of finned surfaces (Fabbri, 1997).

One industrial thermal area in which GAs are extensively used involves power systems, e.g. power plant operation cycle management and cogeneration systems planning. The thermoeconomic models used are typically highly nonlinear. Applications of GAs are sought for the simultaneous optimization of the configuration, design and operation of the installation over its entire economic lifetime by minimizing the time integral of total cost (Olsommer and al., 1997). The GA that allows achievement of such a task combines binary, integer and real encoding and is used on a parallel processor. This large scale optimization shows the incredible possibilities and robustness of GAs.

On the basis of the applications reported above, GAs have been found to be very

powerful optimization procedures. Therefore, in this research these algorithms were investigated for use in designing optimal experiments to determine thermal properties, and in the subsequent simultaneous estimation of the properties. The use of GAs in these areas was particularly sought for the optimization of several experimental parameters and the simultaneous estimation of multiple thermal properties regardless of the presence of correlation among the properties. It is of interest to note that there is no knowledge of previous attempts to use GAs in these areas. The GAs developed in this work were based on real encoding. It should be mentioned here that for the task of optimizing functions of real variables, Evolutionary Strategy approaches have shown some appreciable robustness. However, although they have been around for about 30 years (Schwefel, 1995), these algorithms are still unknown to many investigators and much less theory than for GAs has been developed. Consequently, the ES approach was not investigated in this work.

CHAPTER 3

Parameter Estimation and Design Optimization: Theoretical Considerations

This chapter provides the theoretical tools needed in developing a genetic-based methodology for both experimental design optimization and simultaneous parameter estimation, and in performing the studies reported in Chapters 5 and 6. The inverse methodology for parameter estimation is first introduced, including problem formulation, and presentation and discussion of a popular gradient-based procedure, the modified Box-Kanemasu method. Some important factors to examine are described, namely sensitivity coefficients, correlation matrix, condition number, residuals, root-mean-square error and confidence intervals of the parameter estimates. The second section deals with the methodology for designing optimal experiments to be used for property estimation. The optimization problem is formulated and the main optimality criteria are discussed.

3.1 Parameter Estimation Inverse Methodology

Parameter estimation typically involves the determination of one or more parameters contained in a vector $\boldsymbol{\beta}$. The parameters are inherent in a mathematical model of a measurable (dependent/state) variable, η, of some physical process. In the following, general considerations are provided based on such a variable η which is assumed to be a function of known independent variables such as position and/or time, contained in the vector $\tilde{\mathbf{x}}$. Note that in the thermal characterization problems treated in Chapter 5, the dependent variable is temperature, and the vector $\boldsymbol{\beta}$ contains for instance thermal conductivity and specific heat, while in the kinetic characterization problems treated in Chapter 6, the dependent variable is either the cure rate or the degree of cure of the reaction, and $\boldsymbol{\beta}$ contains kinetic parameters.

3.1.1 Formulation

Parameter estimation can be seen as an optimization in which the objective is to select the values of some unknown parameters in such a way that an objective function is minimized. This latter is specified by the estimator scheme chosen to be applied. The three main estimators, Ordinary Least Squares (OLS), Maximum Likelihood (ML) and Maximum a posteriori (MAP) were introduced in Chapter 2. The objective functions associated with these estimators are expressed by different sum-of-squares functions which contain calculated and measured values of the state variables considered. It is however possible to give a sum-of-squares that is suitable for OLS, ML and MAP estimation when appropriately specialized. In matrix form, this function is (Beck and Arnold, 1977):

$$S(\boldsymbol{\beta}) = \left[\boldsymbol{\eta}(\boldsymbol{\beta}, \tilde{\mathbf{x}}) - \tilde{\boldsymbol{\eta}}\right]^{\mathrm{T}} \mathbf{W} \left[\boldsymbol{\eta}(\boldsymbol{\beta}, \tilde{\mathbf{x}}) - \tilde{\boldsymbol{\eta}}\right] + \left[\boldsymbol{\beta} - \boldsymbol{\mu}\right]^{\mathrm{T}} \mathbf{U} \left[\boldsymbol{\beta} - \boldsymbol{\mu}\right] \tag{3.1}$$

where $\boldsymbol{\beta}$ is the true parameter vector and $\boldsymbol{\eta}(\boldsymbol{\beta}, \tilde{\mathbf{x}})$ and $\tilde{\boldsymbol{\eta}}$ are the modeled and observation vector, which comprise of calculated and measured values of η at specific values of the independent variables contained in $\tilde{\mathbf{x}}$, respectively. Both **W** and **U** are symmetric and square $n_p \times n_p$ matrices, where n_p is the number of unknown parameters. In MAP estimation, **W** is set equal to the inverse of the covariance matrix of the measurement errors, **U** is the inverse of the covariance matrix of the prior information parameters and $\boldsymbol{\mu}$ is the prior information parameter vector. In ML estimation, **W** is the same as in MAP but **U** is set to zero. Eventually, in OLS estimation, no information is assumed and **W** is set to the matrix identity while **U** is set to zero.

Independently of the inverse technique used to minimize *S*, the inverse methodology can be schematized as shown in Fig. 3.1.

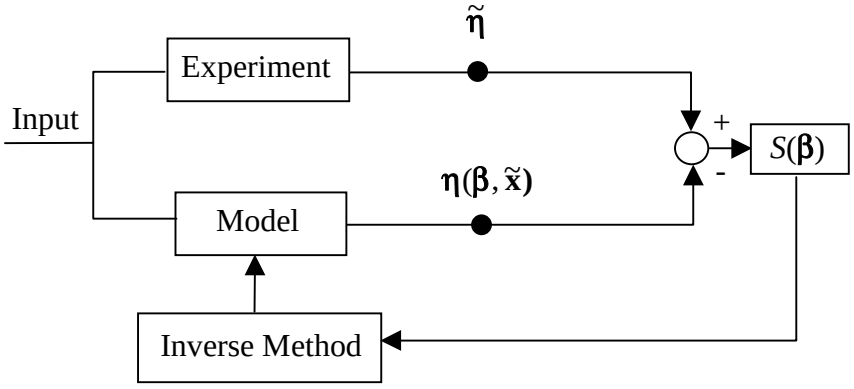

Figure 3.1 Schematic of parameter estimation inverse methodology.

3.1.2 A Gradient-Based Procedure: the Modified Box-Kanemasu Method

- **Description**

Application of a gradient-based procedure as an inverse technique involves setting the derivative of the function *S* with respect to the parameter vector equal to zero:

$$\nabla_{\boldsymbol{\beta}} S = 2\left[-\nabla_{\boldsymbol{\beta}} \boldsymbol{\eta}^{\mathrm{T}}(\boldsymbol{\beta}, \tilde{\mathbf{x}})\right]\mathbf{W}\left[\boldsymbol{\eta}(\boldsymbol{\beta}, \tilde{\mathbf{x}}) - \tilde{\boldsymbol{\eta}}\right] - 2\mathbf{U}\left[\boldsymbol{\beta} - \boldsymbol{\mu}\right] = 0 \tag{3.2}$$

The derivative of $\boldsymbol{\eta}$ with respect to $\boldsymbol{\beta}$ is called the sensitivity matrix and is denoted by $\mathbf{X}(\boldsymbol{\beta})$. Each component of this matrix is a sensitivity coefficient which is associated with a parameter and relates how the dependent variable changes with respect to that particular parameter. Sensitivity coefficients will be discussed in the next section. For nonlinear-in-parameter models (this is the case for all problems investigated in this work) the sensitivity matrix is a function of the parameters, and Eq. (3.2) cannot be explicitly solved for the parameter vector $\boldsymbol{\beta}$. Note that linear estimation implies that the model investigated is of the form $\boldsymbol{\eta}(\boldsymbol{\beta}, \tilde{\mathbf{x}}) = \mathbf{X}\boldsymbol{\beta}$, where $\mathbf{X}$ is independent of $\boldsymbol{\beta}$. Therefore, two approximations are used to linearize Eq. (3.2). The first involves replacing $\mathbf{X}(\boldsymbol{\beta})$ with $\mathbf{X}(\mathbf{b})$, where $\mathbf{b}$ is an estimate of $\boldsymbol{\beta}$. The second uses the first two terms of the Taylor series of $\boldsymbol{\eta}(\boldsymbol{\beta}, \tilde{\mathbf{x}})$ about $\mathbf{b}$ to approximate $\boldsymbol{\eta}(\boldsymbol{\beta}, \tilde{\mathbf{x}})$. These simplifications, along with the use of an iterative scheme (in which the first estimate of $\boldsymbol{\beta}$ could be $\boldsymbol{\mu}$) lead to the following solution for $\mathbf{b}$:

$$\mathbf{b}^{(k+1)} = \mathbf{b}^{(k)} + \underbrace{\mathbf{P}^{(k)}\left[\mathbf{X}^{\mathrm{T}(k)}\mathbf{W}\left[\boldsymbol{\eta}(\boldsymbol{\beta}, \tilde{\mathbf{x}}) - \tilde{\boldsymbol{\eta}}\right] + \mathbf{U}\left[\mathbf{b}^{(k)} - \boldsymbol{\mu}\right]\right]}_{\Delta_g \mathbf{b}^{(k)}} \tag{3.3}$$

where $$\mathbf{P} = \left[\mathbf{X}^{\mathrm{T}(k)}\mathbf{W}\mathbf{X}^{(k)} + \mathbf{U}\right]^{-1} \tag{3.4}$$

Eq. (3.3) is known as the Gauss linearization equation. This method specifies a direction and step size that the parameter vector should be changed in order for *S* to be a minimium. To improve convergence, the Box-Kanemasu modification reduces the step size $\Delta_g \mathbf{b}^{(k)}$ by implementing a scalar interpolation factor *h* which is a quadratic approximation of *S*. Eq. (3.3) then becomes:

$$\mathbf{b}^{(k+1)} = \mathbf{b}^{(k)} + h^{(k+1)}\Delta_g\mathbf{b}^{(k)} \tag{3.5}$$

A further correction modifies *h* to ensure that *S* continuously decreases. The solution for the estimates is obtained when the parameter values do not change significantly from iteration to iteration. For a more in-depth description, refer to Beck and Arnold (1977).

- **Discussion**

Important points about the use of this gradient-based procedure can be made in reference to Eqs. (3.3) and (3.5), and more particularly, regarding the direction of the step size $\Delta_g\mathbf{b}^{(k)}$. First, one can understand that the use of information (matrices **W** and **U**, and vector $\boldsymbol{\mu}$) may help finding a better $\Delta_g\mathbf{b}^{(k)}$ provided this information is appropriate. If the prior information is not in the neighborhood of the final estimates, its use may actually have the opposite effect than its purpose and prevent the method from converging. For that reason, the MAP estimator is usually not used (**U**=0). Using ML and OLS estimators, one can see that the values of the initial estimates should be given great care as they are used to calculate $\Delta_g\mathbf{b}^{(k)}$. Due to the implementation of the scalar factor $h^{(k+1)}$, the modified Box-Kanemasu method offers a little more flexibility in the choice of the initial estimates than the Gauss-Newton method which has been shown to require "good" initial values to be stable. Nevertheless, experience has proven that even the use of the modified Box-Kanemasu method still requires "correct" initial values, e.g. not too far from the neighborhood of the final values.

Two final points worth mentioning are related to the sensitivity matrix and the **P** matrix [Eq. (3.4)]. Obviously, if the sensitivity coefficient of one parameter is negligible, it has some effect on the associated direction and step size for that parameter and thus on the final estimate. In addition, the **P** matrix may also be disrupted from a negligible sensitivity coefficient, thus affecting the estimation of all other parameters. Eventually, unique estimation of the parameters as independent variables is possible only if the **P** matrix exists, e.g. in ML or OLS estimation (**U**=0), the Fisher information matrix defined by $\mathbf{X}^T\mathbf{X}$ is non-singular ($|\mathbf{X}^T\mathbf{X}|\neq 0$, known as the identifiability condition). This implies that the sensitivity coefficients are linearly independent, in other words, not correlated. Note that the condition $|\mathbf{X}^T\mathbf{X}|\neq 0$ also requires that the number of measurements in $\tilde{\boldsymbol{\eta}}$ be equal to or greater than the

number of parameters. This requirement is usually always satisfied in the heat transfer field and in order to minimize the measurement error, it is actually recommended to use a number of measurements at least equal to 20 times the number of parameters (Raynaud, 1999).

In the light of this analysis, considering the use of OLS estimation, application of the modified Box-Kanemasu method requires the following conditions:

1) “correct” initial estimates,

2) sufficient sensitivity information, and

3) uncorrelated parameters.

Note that quantification about conditions 2) and 3) are provided by two respective rules of thumb detailed in the following section. When the three conditions above are fulfilled, then the modified Box-Kanemasu method has been proven to be very effective. But in case these conditions are not met, which characterizes ill-conditioning, the method has been shown to oscillate with increasing amplitude and not converge (Garcia, 1994; Hanak, 1995; Guynn, 1996; and Copenhaver, 1996).

One area in which efforts must be focused prior to the actual implementation of the estimation procedure is the optimization of the experimental design that is used to generate the observation vector $\tilde{\eta}$. Based on an adequate optimality criterion related to conditions 2) and 3), such optimization should facilitate the estimation of the parameters. Optimization of experimental designs is the subject of Section 3.2. However, in the case of very ill-posed estimation problems, it is possible that even after experimental optimization, not only is the sensitivity information still insufficient, but also some parameters are still correlated (Hanak, 1995; Guynn, 1996; and Copenhaver, 1996). Note that Box has actually shown that high correlations among the parameters can be due to a large extent to the nature of the model itself and thus no experimental design could be expected to yield uncorrelated parameter estimates (reported by Beck and Arnold, 1977). In that case, the modified Box-Kanemasu method (and most probably any other gradient-based procedures) is simply ineffective. One solution commonly applied is to follow the principle of parsimony (Beck and Arnold, 1977) that states that the smallest possible number of parameters should be estimated. However, this considerably restricts researchers to estimation of a few parameters by experimental design. In

addition, if the same mathematical model is used, the unknown parameters that cannot be estimated are usually set to nominal values that then introduce a bias in the final estimates. The magnitude of this bias will be a direct consequence of the uncertainty contained in the nominal values, the sensitivity to these values, and the degree of correlation between the parameters to be estimated and the supposedly known one. Therefore, there is a need to develop a methodology capable of solving such ill-defined simultaneous parameter estimation problems. Genetic Algorithms were investigated in this research because they were thought to have this potential. These algorithms are described in the next chapter.

3.1.3 Sensitivity, Correlation and Condition Number Analysis

Of particular interest before starting any estimation procedure is the careful analysis of both sensitivity of the mathematical model to the unknown parameters, and degree of correlation of the parameters. These concepts are important since small magnitudes of the sensitivity coefficients and near-linear dependence among the coefficients are limiting factors to the stability, and thus convergence, of gradient-based estimation procedures, as outlined earlier. In addition, computation of the condition number of the Fisher information matrix $\mathbf{X}^T\mathbf{X}$ can allow assessment of any ill-conditioning characteristic of the estimation problem. In the following, expressions for the sensitivity coefficients and the correlation matrix are detailed and then two rules of thumb that are useful to quantify sensitivity and correlation, respectively, are provided. This section concludes with the mathematical definition of the $\mathbf{X}^T\mathbf{X}$ matrix condition number and its physical signification.

- **Sensitivity**

A sensitivity coefficient, X_β, is defined as the effect that a change in a particular parameter β has on the state variable and is expressed by (Beck and Arnold, 1977):

$$X_\beta = \left.\frac{\partial \eta}{\partial \beta}\right|_{\gamma_i \neq \beta} \tag{3.6}$$

where γ_i are all parameters other than β that remain constant. The larger X_β, the more sensible η is to β and the easier the estimation of this parameter (provided the inverse method converges). In addition, viewing the sensitivity coefficients can allow insight to be obtained

into the adequacy of the mathematical model and that of the experimental design. When performing a sensitivity study, it is meaningful to examine the dimensionless sensitivity X_β^+ given by:

$$X_\beta^+ = \beta \left. \frac{\partial \eta^+}{\partial \beta} \right|_{\gamma_i \neq \beta} \tag{3.7}$$

where η^+ is the dimensionless dependent variable. One convenient and generally appropriate expression for η^+ is:

$$\eta^+ = \frac{\Delta\eta}{(\Delta\eta)_{\max}} \tag{3.8}$$

where $\Delta\eta = \eta - \eta_{\min}$ and $(\Delta\eta)_{\max} = \eta_{\max} - \eta_{\min}$. The term $\eta_{\min}$ is the minimum value of η (which is also the initial value in all problems investigated in this work), while $(\Delta\eta)_{\max}$ is the maximum increase of η between the beginning and end of the experiment. Eq. (3.7) can then be rewritten as:

$$X_\beta^+ = \frac{\beta}{(\Delta\eta)_{\max}} X_\beta \tag{3.9}$$

Whenever the sensitivity coefficients can be solved for analytically, this solution must obviously be selected. However, when no analytical expressions are available, such as when using a numerical model, a numerical alternative must be applied. In this work, the convenient finite difference method was implemented. Note that this method is the numerical alternative recommended by Beck and Arnold. This choice was supported by the fact that on one hand, the inverse estimation methodology developed in this work is based on genetic algorithms which do not use sensitivity coefficients. On the other hand, the finite difference accuracy obtained in computing these coefficients is generally acknowledged to be sufficient for the experimental optimization.

A Taylor series expansion was used to approximate the derivative. To minimize the computational cost, a forward difference approximation (first-order accurate) was chosen which gave for X_β:

$$X_\beta = \frac{\eta(\beta + \Delta\beta) - \eta(\beta)}{\Delta\beta} + o(\Delta\beta), \quad \Delta\beta = \delta \times \beta \tag{3.10}$$

where one can see that the truncation error of the approximation is of order o($\Delta\beta$). Thus a smaller δ (and thus a smaller $\Delta\beta$) would yield a more accurate approximation. However, care has to be taken so as not to make δ too small in order to avoid numerical round-off errors. The work from Tortorelli and Michaleris (1994) indicates that when using single precision, δ values of 10^{-3} and 10^{-4} would provide reasonable accuracy, while when using double precision, accurate results were obtained for δ values of 10^{-4} to 10^{-10}. In addition, the double-precision computations were more reliable, as expected. Although these conclusions are based on the study of a linear elliptic system (which for instance governs linear steady-state conduction), they are nevertheless pertinent here since pertaining to numerical computation. In this work, whenever the finite difference method was used to compute sensitivity coefficients, several perturbation sizes, δ, were tested to verify that reliable results were obtained. Generally, the perturbation sizes used were between 10^{-4} and 10^{-6} using double precision.

- **Correlation**

As mentioned earlier, correlation between the parameters, e.g. linear dependence, plays a critical role in gradient-based inverse methods. One way to investigate correlation is to simply plot the sensitivity coefficients against each other. If they appear to be nearly linear dependent the corresponding parameters are correlated and cannot be estimated simultaneously (Beck and Arnold, 1977). Another way is to plot the sum-of-squares function *S*. Contours that are long, narrow and curving are frequently associated with near-linear dependence. Because plots can often be inconclusive, it is recommended to compute the correlation coefficients, r_{ij}, defined by Walpole and Myers (1993):

$$r_{ij} = \frac{\mathrm{cov}\left(\beta_i, \beta_j\right)}{\sigma_i \sigma_j} \tag{3.11}$$

where σ_i and σ_j are the standard deviations of parameters *i* and *j*, respectively. Assuming the standard statistical assumptions apply, which involve uncorrelated, additive, normally distributed errors with zero mean and constant variance σ^2, errorless independent variables and no prior information regarding the parameters, then the approximate (from linear OLS estimation) covariance matrix of the estimation vector $\boldsymbol{\beta}$ is $[\mathbf{X}^T\mathbf{X}]^{-1}\sigma^2$. Therefore, the

correlation terms, r_{ij}, can be approximated using:

$$r_{ij} = \frac{P_{ij}}{\sqrt{P_{ii} P_{jj}}}, \quad i, j = 1, \ldots, n_p \tag{3.12}$$

where the P_{ij} terms can be found from Eq. (3.4). The r matrix is symmetric with the diagonal terms being unity (obviously, each parameter is completely correlated with itself) and the off-diagonal terms being between –1 and 1. As the magnitude of these terms approaches unity, the properties approach linear dependence. Beck and Arnold (1977) stated that this condition of linear dependence is <u>almost</u> satisfied in the region of the minimum S in many more cases than would be expected. However, because parameters are <u>never completely</u> correlated (provided one uses an appropriate experimental design as defined in Section 2.2.1), the sum of squares error S has a unique minimum point and thus a unique set of parameters. That minimum point may not be very pronounced, however.

It is important to note that unlike linear estimation, Eq. (3.12) is an approximation for nonlinear models, with the approximation being better for cases which are less nonlinear than others. This comment, along with the standard statistical assumptions made above, also applies for all subsequent expressions. Regarding the validity of these assumptions, the residuals analysis (described in Section 3.1.4) is one convenient means to verifying it.

- **Sensitivity and Correlation Quantification**

Two rules of thumb can be used to quantify sensitivity and correlation. One would like:

- the magnitude of the dimensionless sensitivity coefficients to be greater than 0.1, and
- the magnitude of the off-diagonal correlation terms to be lower than 0.9.

Although those values are by no means “exact”, experience has proven that they were pertinent. Indeed, when using traditional gradient-based estimation procedures, lower X^+ than 0.1 and greater r_{ij} than 0.9 usually lead to problems with convergence and resolution of accurate parameter estimates.

- **Condition Number**

The condition number of the Fisher information matrix $\mathbf{X}^T\mathbf{X}$ can be defined as:

$$cond = \frac{|\lambda_1|}{|\lambda_{n_p}|} \tag{3.13}$$

where λ_1 and λ_{np} are the largest and smallest eigenvalues of the $\mathbf{X}^T\mathbf{X}$ matrix (which has a rank n_p), respectively. From this definition, one can understand that a large condition number could come from:

- a large difference between the largest and smallest eigenvalues, which is directly related to a large difference between the highest and lowest sensitivity coefficient magnitudes,
- a very small value for the smallest eigenvalue, which is directly related to a very small value for the lowest sensitivity coefficient magnitude, and
- the presence of linear dependence(s) between the parameter sensitivity coefficients.

The condition number of the $\mathbf{X}^T\mathbf{X}$ matrix can therefore be thought of as a quantification of the illness of the estimation problem. It indicates that, in addition to sufficient sensitivity information and uncorrelated parameters, one wishes to have sensitivity magnitudes on the same order for all parameters. There is unfortunately no rule of thumb for this number. However, the comparison between two condition numbers associated with two different $\mathbf{X}^T\mathbf{X}$ matrices can allow assessment of which matrix, and therefore, which estimation conditions, are the most stable. Notice here, that the condition number is independent of the measurement error.

3.1.4 Residuals and Root-Mean-Square (RMS) Analysis

Two other very important factors in the parameter estimation are the examination of both the residuals and Root-Mean-Square error after the final estimates have been obtained.

- **Residuals**

The residuals are the differences between calculated and observed values of the state variable, that is:

$$e_i = \eta_i(\boldsymbol{\beta}) - \tilde{\eta}_i \ , \quad i = 1, \ldots, N_i \tag{3.14}$$

where N_i is the number of observations taken at a specific sensor. Through the visual inspection of the residuals, one can learn much about the validity of the estimation procedure and of the model. In addition, this examination allows the testing of which assumptions made in the computation of the correlation matrix, RMS, confidence intervals of the final estimates, and in the determination of the optimal design (these concepts which have not yet been discussed will be in the following) seem to be valid regarding the measurement errors. Draper et al. (1981) present a thorough investigation into this subject, emphasizing that plots of the residuals are very illustrative. One would like to have small, centered around zero, and uncorrelated measurement errors. However, often the shape of the residuals contains a "signature", which means that the shape is the same for different experiments and presents few sign changes. This indicates some bias or inconsistency in the mathematical model. Note that the inconsistency may result from inaccurate values used for presumably known parameters (thermocouple position, dimensions, material properties other than those estimated, temperature and heat flux measurements, to name the most relevant). Uncertainties in these latter can indeed have strong effects on the accuracy of the final estimates. Because tests based on data that were used to derive the model can be deceptive and dangerous, of interest is the model testing using a new set of data. That is, the examination of the residuals from an additional sensor whose measurements were not used to compute the sum of squares error *S*. However, this is not always possible, for instance in the case where a numerical mathematical model is used and where measurements from all other sensors are implemented to specify the boundary conditions.

Note that for transient models, the concept of sequential estimation (Beck and Arnold, 1977) in which the parameters are estimated at each time step is also a very convenient means of evaluating the adequacy of the model and that of the design (in addition to the advantage of observing the effects of additional data on the sequential estimates). However, this concept was not utilized in the current work as its implementation into the genetic algorithm

procedure developed was thought to increase the computation cost considerably.

- **Root-Mean-Square (RMS) Error**

The Root-Mean-Square error is defined by

$$\mathrm{RMS} = \sqrt{\frac{S(\beta)}{\left(N_{tot} - n_p\right)}}, \tag{3.15}$$

where N_{tot} is the total number of observations used to compute S; that is for instance, if there are N_i observations from m thermocouples, $N_{tot}=m\times N_i$, while if N_j experiments of N_i observations from only one thermocouple are considered, then , $N_{tot}=N_j\times N_i$. Ideally, the RMS should be small, and usually, the larger N_{tot}, the smaller the RMS (and consequently, the smaller the confidence intervals around the estimates which are discussed next).

When mean thermal property values are computed from a number of different experiments investigated individually, it is common to look at both the $\mathrm{RMS_i}$, which is found for each experiment using the thermal properties estimated for that experiment i, and the $\mathrm{RMS_M}$, which is found using the mean values applied to a particular experiment.

3.1.5 Confidence Intervals (CIs)

Confidence Intervals (CIs) of estimated parameters are used to determine the accuracy of the estimates. For a given nonlinear OLS estimation, assuming the only source of error is the measurement error, the CIs of the individual estimates can be approximated using the formula:

$$\beta_k = b_k \pm t_{1-\alpha/2}(N_{tot} - n_p)\sqrt{P_{kk}\,\frac{S(\boldsymbol{\beta})}{N_{tot} - n_p}} \tag{3.16}$$

where β_k is the predicted property, b_k is an estimate for β_k, P_{kk} represents the k^{th} diagonal term of the **P** matrix, S is the least squares error and t is the student t-distribution for N_{tot}-n_p degrees of freedom and $\alpha/2$ is the confidence range (Walpole and Meyers, 1993). For a large value of N_{tot}-n_p and 95 % probability, $t_{1-0.05/2}(\infty)$ is 1.96 and Eq. (3.16) can be rewritten as:

$$\beta_k = b_k \pm 1.96\text{RMS}\sqrt{P_{kk}} \tag{3.17}$$

The CIs indicated here basically describe the possible amount of variation in the estimates due to, on one hand, the sensitivity of the model to the parameter and the condition number of the Fisher information matrix (through the **P** matrix) and, on the other hand, the resulting RMS. Therefore, inaccurate estimates may come from very small sensitivity of the model to the parameters as well as an ill-defined Fisher information matrix (for instance due to correlation between parameters; see the paragraph about the definition of the condition number and its physical signification) or inadequacy to reproduce the experimental data (possible sources of high residuals have been discussed in the previous section). Recall that this expression is derived for linear-in-parameter models. It is, however, pertinent here to mention the work of Grimstadt and Mannseth (1998) who reported a Monte Carlo analysis that aimed to check the validity of using these approximate CIs for nonlinear estimation. These authors indicate that use of such approximation was almost always justified even for the highly nonlinear model they analyzed

It is advised to check that the CI magnitude agrees with the sensitivity analysis, that is the parameter which has the largest sensitivity coefficient should have the smallest CI. Because of the consideration of the measurement errors only, if the Fisher information matrix is well-defined, the CIs may result in very small value. However, recall that uncertainties in the presumably known parameters have also some effects on the accuracy of the final estimates that may often be much larger than the effect of the measurement errors. For a true measure of confidence in the estimates, uncertainties in the variables set as known should be included (Jarny and Maillet, 1999). Because several different estimation problems were investigated in this research, uncertainties besides the measurement errors were, however, not analyzed and the parameter CIs were simply calculated from Eq. (3.17)

In the case of multiple estimates, the CIs of the mean values of *n* estimates, $\bar{b}_k$, can be computed from two expressions which are (Walpole and Myers, 1993):

$$\bar{b}_k \pm t_{1-\alpha/2}(n-1)\frac{s}{\sqrt{n}} \tag{3.18}$$

$$\bar{b}_k \pm t_{1-\alpha/2}(n-1)\frac{\sqrt{\sum_{i=1}^{n}\frac{s_i^2}{n^2}}}{\sqrt{n}} \tag{3.19}$$

In both equations, t is the value of the t-distribution for n-1 degrees of freedom and $\alpha/2$ is the confidence range. Equation (3.19) is expected to be more appropriate than Eq. (3.18) because it includes the sample standard deviation s_i of each individual experiment [$s_i = \mathrm{RMS}\sqrt{P_{kk}}$ from Eq. (3.17)], whereas Eq. (3.18) assumes the same standard deviation around the mean, s, for the n experiments.

3.2 Design Optimization Methodology

Because all estimators (OLS, ML and MAP) require experimental measurements, the acquisition of data with the most sensitivity for the unknown parameters entails experimental design optimization. In the following, the optimization problem is first formulated. Then, three optimality criteria are described and discussed with an emphasis on the well known *D*-criterion. This section concludes with the need for a robust and reliable optimization technique.

3.2.1 Formulation

In the specific case of optimizing experimental designs used for parameter estimation, the objective is to obtain the greatest possible accuracy; that is, to minimize the variance of the n_p estimated parameters. Consider for an exact (e.g. unbiased) experiment that some observations $\tilde{\eta}_i$ are taken and the seven standard statistical assumptions given in Section 3.1.3 (and denoted 11111-11 in Beck and Arnold, 1977) apply. The $n_p \times n_p$ Fisher information matrix is $\mathbf{X}^T\mathbf{X}$ and the approximate (from linear OLS estimation) covariance matrix of the estimation vector $\boldsymbol{\beta}$ is $[\mathbf{X}^T\mathbf{X}]^{-1}\sigma^2$ (where σ^2 is the assumed equal variance of the measurement error). From this, one understands that the objective function, called the optimality criterion here, should be based on inferential properties of the $\mathbf{X}^T\mathbf{X}$ matrix and, therefore, depends on the sensitivity matrix $\mathbf{X}$. Before describing the main optimality criteria proposed for the design of experiments, one important factor to mention is the intelligent selection of the experimental parameters that are anticipated to have a substantial effect on the model response, and more

particularly on the magnitude of the sensitivity coefficients. The experimental parameters can be associated with the experimental setup as well as with the experimental procedure. Usually boundary conditions, time, and sensor location are the most critical experimental parameters. In addition, one should keep in mind that the optimal experiment should be designed to be experimentally reproduced. Therefore, feasibility of the experimental design (for instance, in implementing particular boundary conditions) should be one priority. Clearly, the closer experiments are to the optimal design, the more accurate the estimated properties will be. This also implies that the standard statistical assumptions are respected as much as possible.

An additional relevant point pertains to the fact that the optimal values determined for the experimental parameters with respect to an optimality criterion should also be appropriate regarding the minimization of the model response sensitivity to the "supposedly" known parameters. As outlined by Raynaud (1999), design-of-experiment should be formulated in terms of two objectives: the maximization of an optimality criterion for the estimation of unknown parameters as well as the minimization of the sensitivity to all other parameters.

3.2.2 Optimality Criterion

- **Description**

The three most often encountered optimality criteria proposed for the design of experiments are the *D*-, *A*- and *E*-optimality criteria. These criteria provide various measures of the size of the confidence region of the estimates. With the assumption that the observations are normally distributed, the confidence region is described by ellipsoids in the parameter space. In addition to the seven standard statistical assumptions, these criteria are subject to some constraints such as maximum duration of the experiments, maximum range of the dependent variable, and large number of observations with uniform spacing in time. Following is a brief outline of their definition and simple geometrical meaning (Kiefer, 1981):

- the *D*-criterion, which is the most commonly used, involves the maximization of the determinant of the Fisher information matrix $\mathbf{X}^T\mathbf{X}$ (or minimization of the determinant of $[\mathbf{X}^T\mathbf{X}]^{-1}$). The determinant of $[\mathbf{X}^T\mathbf{X}]^{-1}$ being proportional to the square of the confidence region hypervolume, *D*-optimality has the effect of minimizing this hypervolume. This criterion therefore minimizes the generalized variance of the estimates.

- the *A*-criterion involves the maximization of the trace of the $\mathbf{X}^T\mathbf{X}$ matrix (or minimization of the trace of $[\mathbf{X}^T\mathbf{X}]^{-1}$). Because the trace of $[\mathbf{X}^T\mathbf{X}]^{-1}$ is proportional to the sum of squares of lengths of the principal axis of the confidence region, *A*-optimality has the effect of minimizing the quadratic average of principal axis lengths. This criterion therefore minimizes the average variance of the estimates.
- the *E*-criterion involves the maximization of the minimum eigenvalue of the $\mathbf{X}^T\mathbf{X}$ matrix (or minimization of the maximum eigenvalue of $[\mathbf{X}^T\mathbf{X}]^{-1}$). The maximum eigenvalue of $[\mathbf{X}^T\mathbf{X}]^{-1}$ being proportional to the square of the maximum diameter of the confidence region, *E*-optimality has therefore the effect of minimizing this maximum diameter.

Obviously, the geometrical and theoretical meaning given here for these optimality criteria is not exact for real estimation problems (nonlinear estimation problems in which the standard statistical assumptions are not satisfied and neither is the “equal spacing” constraint). However, by solving the simpler analogue formulation, one can get an idea on how good (if not optimum) the design can be in more complex form.

The analysis of the effect of these three criteria on the accuracy of the parameter estimates was one of the specific objectives of this research (see Section 5.1.1.6). In dimensionless terms, the maximization of these criteria can be defined as the maximization of:

$$D^+ = \left\| \left[d_{ij}^+ \right] \right\| \tag{3.20}$$

$$E^+ = \min \left| \lambda_i^+ \right| \tag{3.21}$$

$$A^+ = \sum_{i=1}^{n_p} d_{ii}^+ \tag{3.22}$$

where d_{ij}^+ and λ_i^+ are the ij^{th} element and the i^{th} eigenvalue of the dimensionless $\mathbf{X}^T\mathbf{X}$ matrix. The d_{ij}^+ elements can be calculated from:

$$d_{ij}^+ = \frac{1}{t_N \left(T_{\max}^+ \right)^2} \frac{1}{N_k} \sum_{k=1}^{N_k} \int_0^{t_N} X_{ik}^+(t) X_{jk}^+(t) dt \,, \quad i, j = 1, \ldots, n_p \tag{3.23}$$

where T_{max}^+ is the maximum dimensionless temperature being reached at steady state. Note that time could also be dimensionless. The use of both dimensionless terms and the averaging

over the squared maximum temperature allows, on one hand, comparison of competing designs which, for instance, involve different boundary conditions and, on the other hand, results to be obtained for a specific design that can be applicable to any material. When performing the integration over time numerically, one should obviously use the same computational time step to compare competing designs.

- **Discussion**

Now that these optimality criteria have been defined, it is important to stress that the objective behind designing experiments with respect to either *D*-, *A*- or *E*-optimality is related to the size of the confidence region of the estimates only. On no account is possible correlation(s) between the estimated parameters to be minimized. While one wishes to design experiments in which there is minimum correlation as well as maximum sensitivity of the measured variable to changes in the parameters being estimated (which recall correspond to conditions 2 and 3 in Section 3.1.2), this is not possible using one of the three optimality criterion described here. *D*-optimality is recommended because, by minimizing the generalized variance of the estimation vector, it allows the most accurate global estimation. However, it is possible that a *D*-set of final estimates might be more correlated (while globally more accurate) than a set of estimates obtained from a different design than the *D*-optimal. This will actually be the result of the analysis performed in Section 5.1.1.5. Accuracy and correlation are two different concepts which have been long associated because of the use of gradient-based methods that cannot operate properly in the presence of correlation. However, correlation is simply a characteristic between parameters and it is inherent to the mathematical model investigated, as stressed by Box and reported by Beck and Arnold (1977).

One criterion that one could think of as both maximizing the accuracy of the estimated parameters (by maximizing their sensitivity coefficients) and minimizing the correlation between them is the condition number of the Fisher information matrix $\mathbf{X}^T\mathbf{X}$. However, there is no mathematical proof that minimizing this number would guarantee such output. Besides, Alifanov et al. (1995) have reported that *D*-optimality was nearly equivalent as an optimality criterion based on the $\mathbf{X}^T\mathbf{X}$ condition number. Finally, results of Section 5.1.1.5, for instance, will show that it is possible to obtain for a specific *D*-optimal design a globally more accurate

set of estimated parameters which indicates higher correlation terms between the parameters but, more important, a lower condition number than for a non-optimal design.

One important point to realize in design optimization is that as models are usually nonlinear, the sensitivity coefficients depend on the unknown parameters. Therefore, an iterative design optimization must be implemented. Such iterative scheme consists in 1) performing the optimization using initial estimates for all unknown parameters, 2) conducting the experiments as prescribed from the optimal design, and 3) generating estimates from the parameter estimation inverse method. If the new estimates from the experiments are found to be completely different than the previous values used, the optimal parameter settings have to be redetermined. As one can easily guess, for time-consuming direct models, this iterative procedure cannot be rigorously followed. One useful output that has been typically found is that the optimal values for the design variables often lie within an optimal range. This means that the use of initial estimates of the unknown properties different than their actual values may allow for nearly the same optimal design variable values [provided the initial guesses used are not much different than, say, 100 % of the actual final estimates (Moncman, 1994; present study)]. Therefore, the initial estimate values do not have to be exactly the true estimates.

One final point deals with the optimization of a particular parameter, the overall total experimental time. A usual and convenient means to find the optimal setting for this parameter is to calculate a modified value of the optimality criterion chosen once the other experimental parameters have been optimized by maximizing the actual optimality criterion (using an optimization technique). The modification considered consists of computing the criterion without averaging the integral contained in Eq. (3.23) over time. When the modified value of the criterion does not change any more in time, it indicates that little additional information is being provided for the estimation of the parameters and thus the experiments can be concluded. The corresponding time is the value for the overall total experimental time. Note that usually a conservative value is selected.

3.2.3 Optimization Technique

The determination of the optimal experimental variables which satisfy the optimality criterion chosen for the objective function is performed through the application of an optimization technique. As reported in Chapter 2, the typically used parametric study presents drastic drawbacks. On this basis, the use of a robust and reliable method is necessary. The development of an experimental design optimization methodology based on Genetic Algorithms was one of the overall objectives of this work. These algorithms are described in the next chapter.

CHAPTER 4

Genetic Algorithms

This chapter focuses on an emerging evolutionary method called Genetic Algorithms (GAs). After a brief introduction, as GAs were already introduced in Chapter 2, the following section is devoted to presenting the fundamentals behind these algorithms. Next, the three algorithms developed throughout this work are described and discussed. Eventually, this chapter concludes with the demonstration of the robustness of the third GA developed on the optimization of a mathematical test function.

4.1 Introduction

Traditionally, there are two major classes of optimization algorithms which are classified into calculus-based and enumerative techniques (Goldberg, 1989). Calculus-based optimization techniques employ the gradient-directed searching mechanism, starting from an initial guessed solution, and therefore are local in scope. Although these techniques are well developed, they maintain significant drawbacks. Indeed, for ill-defined or multimodal objective functions, instability and/or local optima are usually obtained. In addition, because the objective function is often problem-oriented, implementation of these techniques can be very complex. Many enumerative schemes have been suggested to handle the local optima problem but at the expense of computational inefficiency. A third class that has achieved increasing popularity is the random/probabilistic search algorithm. More particularly, the 1970's has seen the emergence of evolutionary algorithms which employ mechanisms of natural selection to solve optimization problems (Michalewicz, 1996). These algorithms were thought of as the answer to the question of how the search should be organized so that there is

a high likelihood of locating a near-optimal solution. Genetic Algorithms are today the most widely used evolutionary algorithms.

4.2 Fundamentals

The purpose here is not to give a thorough theoretical analysis of the GAs mechanism, as there are excellent introductory tutorials in the literature (Goldberg, 1989; Davis, 1991; Michalewics, 1996; and Mitchell, 1996). There is also *The Hitch-Hicker's Guide to Evolutionary Computation* available on the internet (Heitkoetter and Beasley, 1994). Instead, the objective of this section is to provide some answers to explicit questions one may have about GAs. In the following, the structure of a simple GA will be presented along with a general overview of the main techniques/variants that are employed in the GA process. Then, the most important features which differentiate GAs from conventional optimization techniques are described. Eventually, the strengths and weaknesses of GAs are outlined and the type of problems for which the use of these algorithms is pertinent is indicated.

4.2.1 What Are GAs?

Like all evolutionary algorithms, a GA is a search procedure modeled on the mechanics of natural selection rather than a simulated reasoning process. Developed by Holland (1975), these algorithms were originally used for the study of artificial systems. Since their inception GAs have been subject to a growing interest as an optimization technique in nearly all kinds of engineering applications. Today, there are so many different GAs that it turns out, as Mitchell states (1996), that there is no rigorous definition of GAs accepted by all in the evolutionary computation community that differentiate GAs from other evolutionary computation methods. Indeed, some currently used GAs can be very far from Holland's original conception. However, it can be said that most methods called "GAs" have at least the following elements in common: populations of individuals, selection according to the individuals' fitness, crossover to produce new individuals, random mutation of new individuals, and replacement of the populations. These elements are illustrated next, in the description of how a simple GA works. A typical GA flowchart appears in Fig. 4.1.

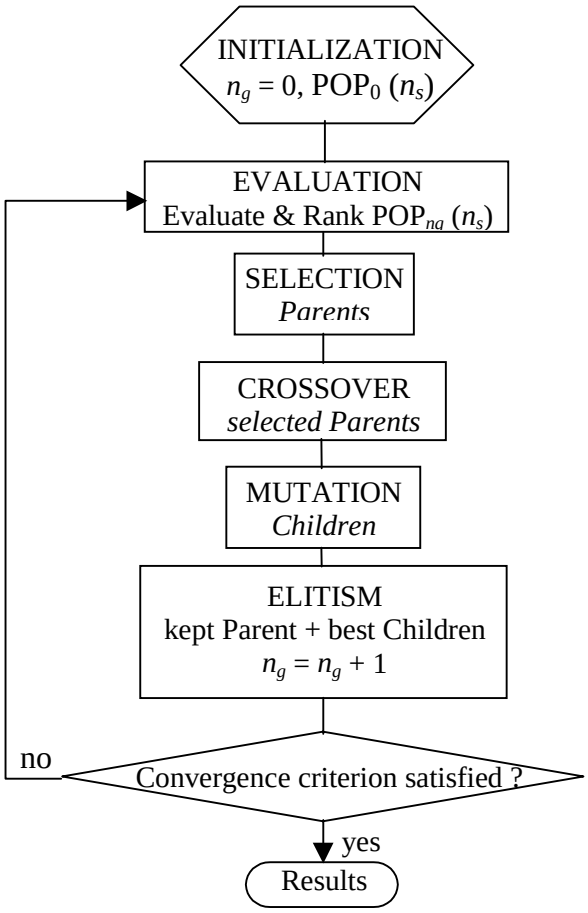

Figure 4.1 Typical Genetic Algorithm flowchart.

4.2.2 How Do GAs Work?

GAs are based on the collective learning process within a population of individuals (trial solutions called chromosomes), each of which represents a search point in the space of potential solutions to a given problem. The chromosomes code a set of parameters (called genes). The population (of size n_s) is generally randomly initialized (at the generation n_g=0) in the parametric search space (see POP$_0$ in Fig.4.1). The individuals are evaluated and ranked in terms of a fitness function. Then, the population evolves towards fitter regions of the search space by means of the sequential application of genetic operators. The basic operators of a simple GA consist of selection (selection of parents for breeding), crossover (mating of parents to create children) and mutation (random changing of a gene). Following the Darwinian theory of survival of the fittest, an elitism operator is usually found in the generational replacement. A generation is accomplished when the sequence defined by the application of all operators to the individual parents is performed, as illustrated in Fig. 4.1.

The GA produces as many generations as necessary until the convergence criterion is reached. The goal, throughout this process of simulated evolution, is to obtain the best chromosome in the final population to be a highly evolved solution to the problem.

The main techniques/variants that are employed in the GA process for encoding, fitness evaluation, parent selection, crossover, mutation, replacement and convergence are reviewed next.

4.2.3 What Are the Main Operator Variants Employed in the GA Process?

The genetic operators have all several variants which can be applied in a randomly and/or probabilistic (sometimes deterministic for some algorithms) process. These variants may be quite specific in single applications but a number of standard variants are used by most GAs. The following paragraphs briefly review the main standard genetic operator variants. Again, note that it is not intended to give descriptions of all variants mentioned, as the literature cited earlier provides excellent details about all. However, when describing the GAs developed (Section 4.3) the variants used will be explained. Figure 4.2 introduces the general structure of a standard simple GA (based on Fig. 4.1). In addition, as an introductory tutorial, the mechanisms behind the genetic operator variants of such a simple GA are developed in Appendix A using a simple function optimization example.

- **Description**

Encoding Scheme

To enhance the performance of a GA, a chromosome representation that stores problem-specific information is desired. Although GAs were developed to work on chromosomes encoded as binary strings (Fig. 4.2), it is today common knowledge that for numerical optimization problems, one should use a GA with floating point representation. One important point that may, however, not be obvious when one starts to use GAs (which was my case) is that the crossover variants used should be appropriate to the encoding used. There indeed exist both conventional (binary) and arithmetical crossover techniques to fit the two different representations. Note that when using the real representation, a chromosome is a vector of n_p genes for the n_p parameters. It should be emphasized here that because much of the early work of GAs used a universal coding involving abstract binary chromosomes (that needed to be

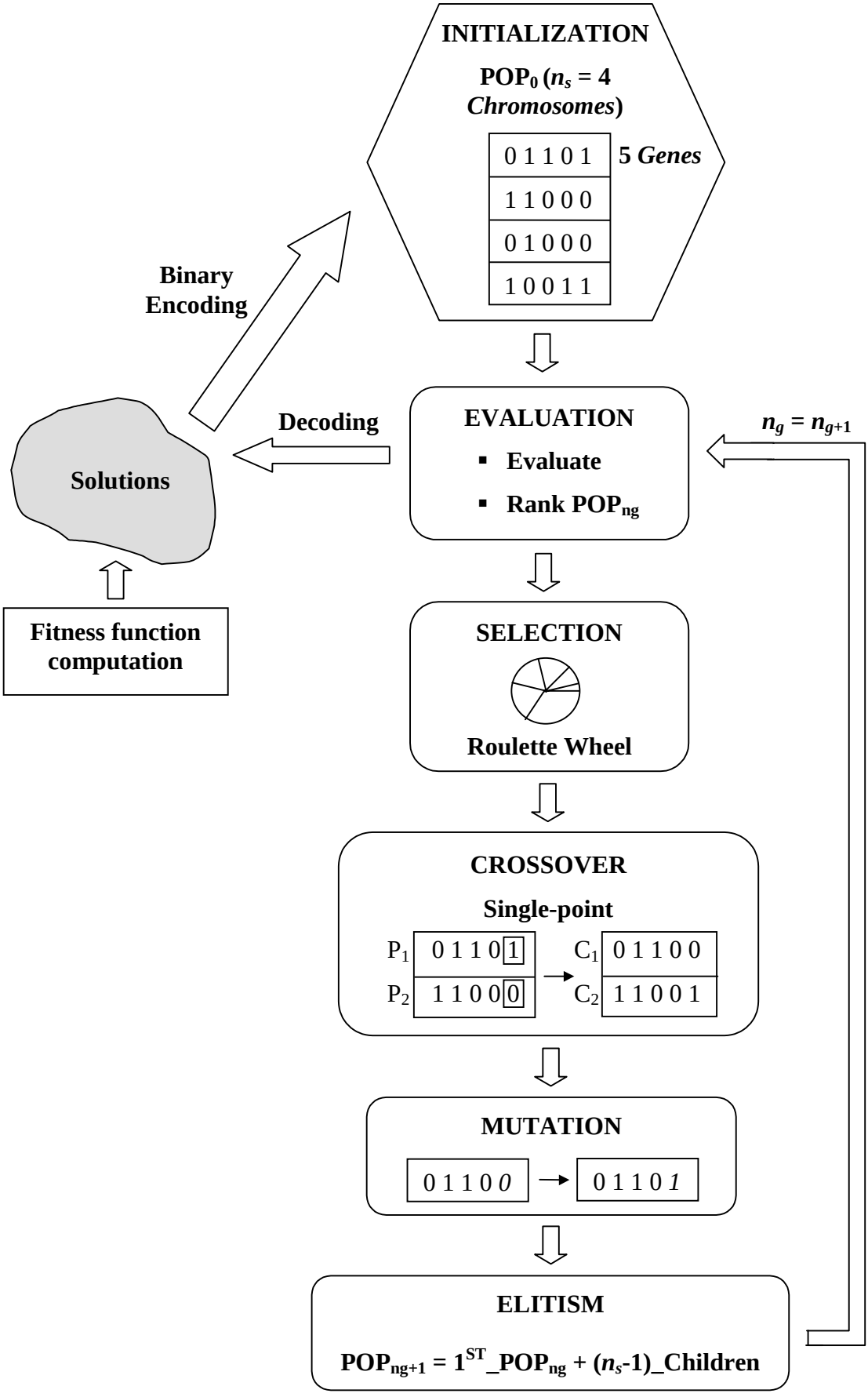

Figure 4.2 General structure of a standard simple Genetic Algorithm.

decoded), research on GAs has been slow to spread from computer science to engineering, and very little theory exist in the literature on real-valued encoding.

Fitness Function

The fitness plays the role of the environment in which the chromosomes are to be evaluated (Fig. 4.2). This is thus a crucial link between the GA and the system. This function can be simply taken as the objective function to optimize or as a transformation (scaling) of it. It is assumed that the fitness function to be optimized is positive. In cases where the objective function happens to be negative, the fitness function will be a transformation of the objective function.

Parent Selection

Basically, the selection operator determines which of the individuals in the current population (of size n_s) will be allowed to pass their genetic material to the next generation. Using the GA language, one says that it builds up the mating pool by selecting n_s individuals from the current population. There are many ways to achieve effective selection, including proportionate, ranking and tournament schemes. The key assumption is to give preference to fitter individuals. Using fitness proportionate selection, the number of times an individual is expected to reproduce is equal to its fitness divided by the average of fitnesses in the population. The most popular and easiest mechanism is the roulette wheel selection (Fig. 4.2) where each chromosome in the current population has a roulette wheel slot sized in proportion to its fitness. However, depending on the environment (fitness), proportionate and ranking selection schemes may lead to premature convergence or on the contrary, to a slow finishing. Those are well-known severe technical problems of GAs. However, both problems can be avoided if scaled fitness values are used instead of the original values. Another way to circumvent these problems is to use a more adequate selection operator. In many applications, tournament selection has proved to yield superior results to fitness rank selection. In the simplest form, the so-called binary selection, two chromosomes are selected randomly from the current population but only the one with the higher fitness value is inserted into the mating pool with a probability p_t. One interesting feature about this selection scheme is that one can adjust the selection pressure directly from the tournament probability p_t (typically larger than 0.5). Regardless of which selection technique is used, the selection operator produces an intermediate population, the mating pool, which consists only of individuals that are members

of the current population. The following two operators, crossover and mutation, are then applied to this mating pool in order to generate children.

Crossover

The crossover operator is the key operator to generate new individuals in the population. Note that the fact that the use of crossover increases the performance of a GA has been proved by two theories, namely the Holland's Schema Theorem (1975) and the Goldberg's Building Block Hypothesis (1989). In addition, it has been shown that so-called "deceptive" problems (Goldberg, 1989) can be made "easy" by the use of an appropriate definition of the crossover function. This operator is applied to each pair of the mating pool with a crossover probability p_c, usually taken from [0.6,1], to produce one or two children. With probability 1-p_c, no changes are made to the parents (they are simply cloned), but with probability p_c, genetic material is exchanged between the two parents. In the simplest crossover, the single point crossover (Fig. 4.2), a crossover point is randomly selected and the portions of the two chromosomes beyond this point are exchanged. Multipoint crossover is similar except that multiple cross points are chosen at random with no duplication. Uniform crossover generalizes the scheme by making every gene a potential crossover point. Single, multipoint and uniform crossovers are generally considered conventional binary techniques, and when real encoding is used, arithmetic crossovers are the most suited.

Mutation

This operator should allow a GA the finding of solutions which contain genes that are non-existent in the initial population. It can also prevent the GA from loosing some genetic material without any chance of adopting it again. Often viewed as a background operator, mutation modifies gene values according to a mutation probability. Using binary encoding, this simply means changing a 1 to a 0 and vice versa with a small probability (Fig. 4.2). Using real encoding, when a global modification called jump mutation is applied, each gene in any chromosome is replaced with a random value (from the entire parametric search space) with probability p_{mj}. A "mutation-based" operator can also be applied locally with the creep variant (not a pure mutation operator in the sense of GAs) which consists in the addition or subtraction with probability p_{mc} of a small value to the gene (1% of the actual gene value). Whereas the crossover operator reduces the diversity in the population, the mutation operator increases it again. The higher the mutation probability, the smaller is the danger of premature convergence. A high mutation probability will however transform a GA into some kind of

random search algorithm, which is of course not the intention of the algorithm! Mutation probabilities are usually small (so as not to interfere with the combination of the best features of parents made by the crossover operation), and range from 0.001 to 0.10, the higher values being typically applied with real encoding.

Replacement Strategies

In the simplest form of GAs, when the operation of selection, crossover and mutation are completed on the n_s individuals of the current population, this entire population is replaced with the children created. This is the traditional generational replacement. Variations where not all individuals are replaced in each generation exist. The simplest case of such a strategy is the elitist strategy where the individual with the highest fitness (according to the Darwinian theory of survival of the fittest) is directly transferred from the old to the new generation and only the other n_s-1 children are generated by the application of genetic operators (Fig. 4.2). Generational replacement with probability p_r is often used in which $n_s \times p_r$ parents are replaced with children while the $n_s \times (1-p_r)$ best parents are kept. An alternative to replacing an entire population at once is to replace one organism in the population whenever a new organism is created. This variant is known as a steady-state GA.

Convergence Criterion

The most widely used stopping conditions are either that a given number of generations have been done already, or that the population has become uniform. When the first condition is chosen, GAs are typically iterated for anywhere from 10 to 500 or more iterations. User-defined convergence criterion that are better suited to the problem being solved should be preferred (although most of the studies do not address this problem). It is however not easy to define such a criterion, as it will be shown in this work.

Performance Criteria

What does it mean for a GA to perform well or poorly? Some performance criteria can provide answers to this question. The best fitness reached (best-so-far) is a typical one. One criterion for computational cost is the number of function evaluations. Indeed, in almost all GA applications, the time to perform a function evaluation vastly exceeds the time required to execute other parts of the algorithm (which are thus considered to take negligible time). Note that because randomness plays a large role in each run (two runs with different random number seeds will generally produce different output), often GA researchers report statistics

(about the best fitness for instance) averaged over many different runs of the GA on the same problem.

Besides the genetic operators presented here, there exist a number of different operators (inversion, reordering), in addition to advanced features (diploid, dominant and recessive genes, sharing fitness function) which are used in different applications but not yet widely. GAs are still far from maturity.

- **Discussion**

Undoubtedly, GAs possess the attributes of a probabilistic search technique for the global optimum, while it is unfortunately often referred to as a randomized search. It is important to realize that the global optimum solution will not be found in one GA run. GAs are however robust in producing near-optimal solutions, with a high degree of probability to obtain the global optimum (Kroittmaier, 1993).

One may realize at this point that the main challenge in constructing a general-purpose GA programming environment is the selection of the genetic operator variants from the diversity of adaptive techniques that exist, as well as the settings of the genetic parameter values (population size, selection, crossover and mutation probabilities, which could be called “fine tune” parameters as they play a decisive role in the GA success). Indeed, GAs using binary representation and single-point crossover and binary mutation are robust algorithms but are never the best algorithms to use for any problem. There are unfortunately few heuristics to guide a user in the selection of appropriate operators and genetic parameter settings for a particular problem. What can be grasped from the literature is that good GA performance requires the choice of a moderate population size, a high crossover probability and a low mutation probability (for instance, inversely proportional to the population size in using real encoding). This lack of heuristics is a well known problem in GAs. With some experience, one may have an idea about which variants and “right” values to use. Note that such a procedure could be compared with the choice of a numerical scheme and then the grid discretization and number of iterations to apply when using a numerical formulation to solve, for instance, a heat transfer problem.

There are, however, two important issues in GAs that one should use as a guide (this is what I realized before developing the third GA): exploiting the best solutions and exploring the search space. On one hand, the selection operator associated with the fitness function

gives the tendency between exploitation and exploration and is therefore very important. It is usually considered the evolution operator. On the other hand, crossover and mutation are classified as search operators. The first allows both exploitation and exploration, while the second concentrates on exploration. The elitism operator can be viewed as a preservation operator which exploits the best solution(s). As one may guess, a GA efficiency consists of an adequate balance between exploitation and exploration.

4.2.4 What Differentiates GAs From Conventional Techniques?

GAs differ from conventional optimization and search procedures in several fundamental ways. Goldberg (1989) has summarized these as follows:

1. GAs work with a coding of solution set, not the solutions themselves; note that this remark applies particularly more to binary encoding.
2. GAs search from a population of solutions, not a single solution.
3. GAs use payoff information (fitness function), not derivatives or other auxiliary knowledge.
4. GAs use probabilistic transition rules, not deterministic rules.

4.2.5 What Are the Strengths and Weaknesses of GAs?

- **Strengths**

There are major advantages of applying GAs to optimization (or estimation) problems. Easily programmed, GAs are derivative-free calculations and therefore, are neither bound to assumptions regarding continuity, nor limited by required prerequisites. As Goldberg stated, GAs are blind. They can handle any kind of objective function and any kind of constraints (e.g., linear or nonlinear) defined on discrete, continuous or mixed search spaces. In addition, as stated earlier, they are robust in producing near-optimal solutions, with a high degree of probability to obtain the global optimum. Another strength of GAs is their flexibility to be parallelizable and hybridized with other techniques. A parallel GA operates on multiple population pools; whenever computer facilities offer the use of several processors, such a GA can allow for powerful runs. A hybrid search combines local search with a GA. It is an interesting alternative wherein a number of promising initial solutions generated during the GA search are used as the starting point for a locally convergent optimization algorithm.

Davis (1991) advocates hybridization of GAs with domain-specific techniques, usually the ones that were typically used for the problem being investigated. Hybrid GAs are believed to have potential for ill-conditioned inverse problems, and the development of such procedure is actually one of the recommendations of this work (see Chapter 7). Note that hybrid GAs however lose some of their general robustness as they become more specific to the problem at hand.

- **Weaknesses**

Although the GA is a powerful optimization tool, it does have certain weaknesses in comparison to other optimization techniques. A poorly designed GA can perform nearly as badly as a random search. In short, because a GA's performance is highly application-specific, it must be adapted to the task on hand (Davis, 1991). Furthermore, a GA application is sometimes more an art than a science. Besides, due to the randomness part of the GA operations, it is difficult to predict its performance. The success of a GA and its effectiveness in any application can only be determined by experimentation. Another significant drawback is the high CPU cost involved.

4.2.6 For Which Type of Problems Should GAs be Used?

In the light of their strengths and weaknesses, one can guess that for unimodal functions that are smooth, there is no sense in using GAs. Rather, the use of these algorithms seeks to "solve" problems that are intractable with classical procedures. The mathematical function **f6** described in Section 4.4.1 shows the kind of complicated problems a GA can be called upon to solve. Typically for a GA to be used, the design space is large (for instance in the optimization of complex experimental designs), multi-modal, noisy, and fraught with discontinuities. Their use over traditional gradient-based optimization techniques also finds its rationale for problems where the gradient information leads to instabilities (for instance in ill-posed parameter estimation problems). Indeed, because GAs do not require gradient information, but only the computation of values of the objective function to optimize, when applied to parameter estimation problems these algorithms are therefore not limited by correlations that may exist between the parameters. Consequently, GAs provide a general powerful approach to inverse problem solving, in which a good numerical model of the direct problem and a representation for potential solution are the only prerequisite. In addition, it is

relevant to recall here that the use of gradient-based methods for nonlinear estimation necessitates the linearization of the model (see Section 3.1.2). This is not the case when applying GAs.

Note that because there are so many different GAs, many open questions exist about the type of problems for which GAs are best suited and, in particular, the type of problems on which they outperform other search algorithms.

To conclude this section, it should be mentioned that GAs and gradient-based methods should not be considered competing approaches but instead, whenever possible, should work together as these two types of techniques are believed to be complementary. This comment goes along with the advocacy of Davis (1991) to hybridize them (refer to the previous section for an explanation of hybrid GAs). Davis has shown that hybridization of these techniques can lead to better performance than using any of them in isolation.

4.3 GAs Developed

With an aim toward overcoming the limitations of traditional techniques used in experimental design optimization and simultaneous parameter estimation (described in Chapter 3), the main features of Genetic Algorithms (with real encoding) were thought to be exploited and applied to both fields. With very little theory on real encoding existing in the literature, three “GAs” have been developed in this work, each time improving the last version over the previous one. This research has started with a standard GA featuring a Basic Elitist strategy (BEGA) and then it was improved by implementing an Extended Elitist strategy (EEGA) following as much as possible the Darwinian principle of survival of the fittest. Eventually, from the knowledge gained in the GA field, a third GA was developed in which genetic operators more appropriate for real encoding were used, and a convergence criterion was implemented. These three algorithms are successively described next.

4.3.1 Basic Elitist GA (BEGA)

- **Description**

The first GA developed, which was modeled according to the algorithm described by Furuya and Haftka (1993), was called Basic Elitist GA (BEGA) because it used a basic elitist strategy. A detailed description of the BEGA is given here for the particular case of the optimization test problems treated in Section 5.1.1. Note that a single chromosome thus designates a vector of design variables. A simplified flowchart of the BEGA is shown in Fig. 4.3.

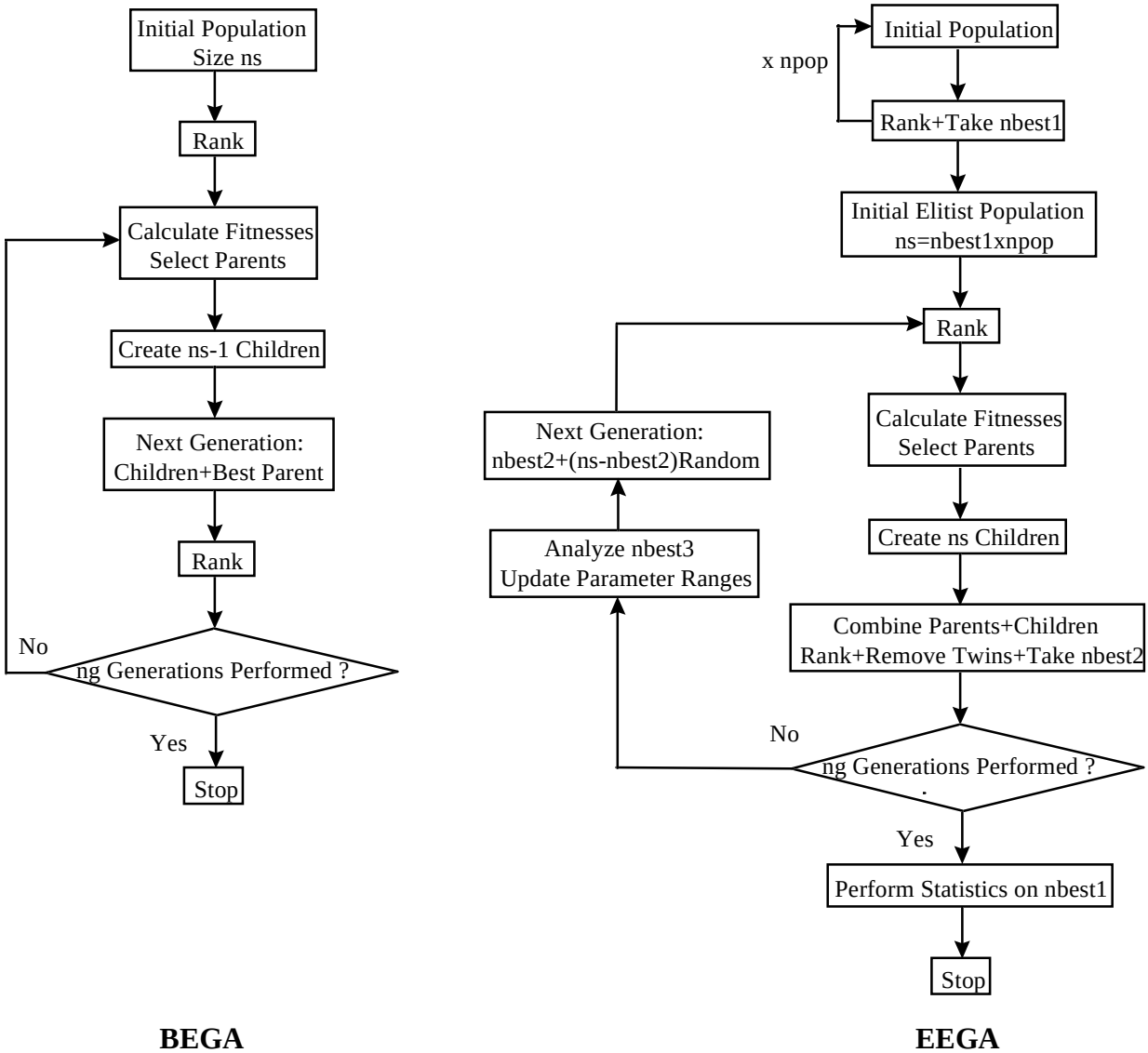

Figure 4.3 Flowcharts of BEGA and EEGA.

Design Coding

In the optimization of the one-dimensional experiment (Fig. 5.1), a chromosome describing a particular design contained two genes for the sensor location x_s^+ and the heating time t_h^+. Along the same lines, in the optimization of the two-dimensional experiments (Fig. 5.2), each chromosome contained four genes for the design variables x_s^+, y_s^+, L_p^+ and t_h^+. The ranges of the real genes depended on the lower and upper bounds of the design variables which were specified by the experiments. For instance, the chromosome x_s^+ (dimensionless sensor location perpendicular to the fibers) ranged from zero to one.

Initial Population

The optimization algorithm started by generating the initial parent population of n_s candidate chromosomes (designs). Each individual was created by randomly selecting n_p gene values (design variable) from the design space. The chromosomes were then ranked in terms of the value of the dimensionless determinant D^+ using the *D*-criterion. Obviously, the best string had the highest D^+.

Selection

Parents were selected by pairs for breeding using a proportionate rank-based fitness technique. The fitness of the i^{th} ranked chromosome was defined as $f_i = n_s + 1 - i$ allowing for the highest ranked chromosome to have the highest fitness parameter and thus to be most likely to contribute to the determination of the next generation strings. The probability of the i^{th} ranked chromosome to be selected as a parent was given by $p_i = \dfrac{2f}{n_s(n_s+1)}$. The selection process was then accomplished at random, according to the roulette wheel mechanism: the i^{th} ranked chromosome was selected if $P_{i-1} \le R \le P_i$, where $P_i = \sum_{j=1}^{i-1} p_j$ and R was a uniformly distributed random number between zero and one.

Crossover

The children were made by the mating of the ($2n_s$) pairs of parents selected for breeding according to the single-point crossover (with a crossover probability p_c of 1.). Note that the simplest crossover operation was chosen to be used because the primary goal using the BEGA was to test the effectiveness of GAs comparatively to the parametric study in the optimization

of experimental designs. This process began by generating a random integer k, the cut-off point, between 1 and n_p-1, where n_p was the number of genes. A child was designed by using the first k genes of parent 1 and the remaining ones came from parent 2 (see App. A). For instance, consider in the one-dimensional analysis the chromosomes with x_s^+=0.5, t_h^+=1.0 and x_s^+=0.7, t_h^+=1.5 as parents 1 and 2, respectively. As n_p=2 (recall that there are two design variables in the one-dimensional analysis), the only possible child chromosome (one child per pairs of parents) could be x_s^+=0.5, t_h^+=1.5.

Mutation

Jump mutation was implemented by changing at random the value of a gene. This process ensured that new genes were generated, thus preventing the solution from locking on a non-optimum value. The mutation probability p_m was taken arbitrarily as 0.05. If the gene was mutated, it was replaced by another one randomly chosen from the allowable range of values for that gene.

When the operations of selection, crossover and mutation were completed on the n_s parent population, a new generation was created from the n_s-1 child chromosomes in addition to the best parent chromosome. This addition denotes the basic elitist strategy of the BEGA. Over the course of several generations, the algorithm tended to converge on the chromosome giving the maximum determinant, which was hence considered as the predicted optimal design. Note that the stopping criterion was simply to perform n_g generations. The number of function evaluations f_{eval} was calculated from $f_{eval} = n_s \times \left(n_g + 1\right)$.

- **Discussion**

The results obtained using the BEGA (see Section 5.1.1.4) showed that this algorithm was limited when the objective function was highly expensive to calculate (two-dimensional design optimization case). More precisely, the optimization method using the BEGA tended to be as time intensive as the parametric study, although it resulted in improved efficiency and was less tedious to apply.

4.3.2 Extended Elitist GA (EEGA)

- **Description**

The second algorithm was developed to improve the efficiency of the BEGA. It used the same genetic operators as the BEGA but with an extended elitist strategy and was thus called Extended Elitist GA (EEGA). Following is an outline of the five main differences between the EEGA and the BEGA. These differences can also be viewed in the simplified flowcharts shown in Fig. 4.3. The EEGA was applied to both the optimization and estimation test problems treated in Section 5.1.1, in addition to the estimation of the thermal and radiative properties of an insulative material (not reported in this dissertation but which can be found in Garcia et al., 1998).

1. A pure random search was initially performed to obtain appropriate starting conditions for the lower and upper bounds of each gene (parameter to be optimized/estimated). The purpose of this seeding was, therefore, to help direct the GA search. Note that this initial search was run separately from the EEGA run.
2. The EEGA started by a successive random search for a number of n_{pop} initial subpopulations in which only the n_{best1} first ranked chromosomes were kept within each subpopulation. This produced an initial elitist population of size $n_s = n_{pop} \times n_{best1}$. (Note that by carefully selecting the parameter space, steps 1 and 2 are comparable to the use of *a priori* information).
3. n_s children were created according to the BEGA and then combined with the parent population. After ranking this combined population of size $2n_s$, the "twins" were removed (usually a small number much lower than n_s) and only the n_{best2} first ranked chromosomes were kept, where $n_{best2} < n_s$.
4. The parameter ranges were updated from the analysis of the n_{best3} first ranked chromosomes, where $n_{best3} \leq n_{best2}$. Additional random chromosomes numbering (n_s-n_{nest2}) were then generated from the just updated parameter ranges and were added to the n_{best2} first ranked chromosomes to form the next generation. By allowing some "new blood" to be brought into the population, population diversity is preserved, therefore preventing, it is thought, the EEGA from premature convergence on a non-optimal chromosome. This feature was also thought to compensate for the use of only the simple

single point crossover which did not produce new gene values.

5. Steps 3 and 4 were repeated until n_g generations had been achieved, and then the means and the 95% confidence intervals [Eq. (3.18)] for each gene were determined for each of these n_{best1} chromosomes. These confidence intervals were a good means of evaluating the convergence of the EEGA. Note that the number of function evaluations was now given by $f_{eval} = \left(n_{pop} \times n_s\right) + \left[n_s + \left(n_s - n_{best2}\right)\right] \times n_g$.

It is important to note that when EEGA was used as an estimation procedure, the output for a particular experimental data set included the means of each gene (thermal property) and the approximate 95% confidence intervals representing the ranges of values which the actual properties lay within for that particular experiment. The calculation of this confidence interval was described in Section 3.1.5 [Eq. (3.17)].

- **Discussion**

The results obtained using the EEGA on the test problems (see Section 5.1.1.4) showed that this algorithm outperformed both the BEGA and the parametric study. However, when applied to the estimation of the thermal properties of an insulative material (Garcia et al., 1998) in which the objective function (least-squares error) presented a "local minimum plain" and a "global minimum valley" on the same order of magnitude, the EEGA tended to direct the search to the local plain at the expense of global perspective. This was the output from the use of the extended elitism strategy which resulted in a strong forced evolution feature preventing the GA from performing a good balance between exploitation and exploration. The removing of twins and the addition of random "blood" were not sufficient to keep a diverse population and prevent a *super chromosome* from dominating the population which then caused premature convergence. In addition, the use of the simple single-point crossover (originally designed for binary encoding) was simply too poor with real encoding as it could not allow new genes to be created.

Based on both the BEGA and EEGA behavior analysis, a third GA was developed. Two main prescriptions were taken into account which were:

1. Elitism should be used cautiously in adequacy with the objective function landscape.

2. One cannot use a naïve simple GA and modify it by implementing all kinds of (elitism) features to make it work properly. Rather, one should use from the beginning an adapted GA to the problem being solved. In my case, this implied to use genetic operators adapted to a real-number encoding.

4.3.3 Third GA (GA_3: GAMAIN and GACONDUCT)

- **Description**

Figure 4.4 illustrates a simplified flowchart of the GA_3. Some of the genetic operator variants were defined in Section 4.2.3. Note that in the problems treated using the GA_3 in

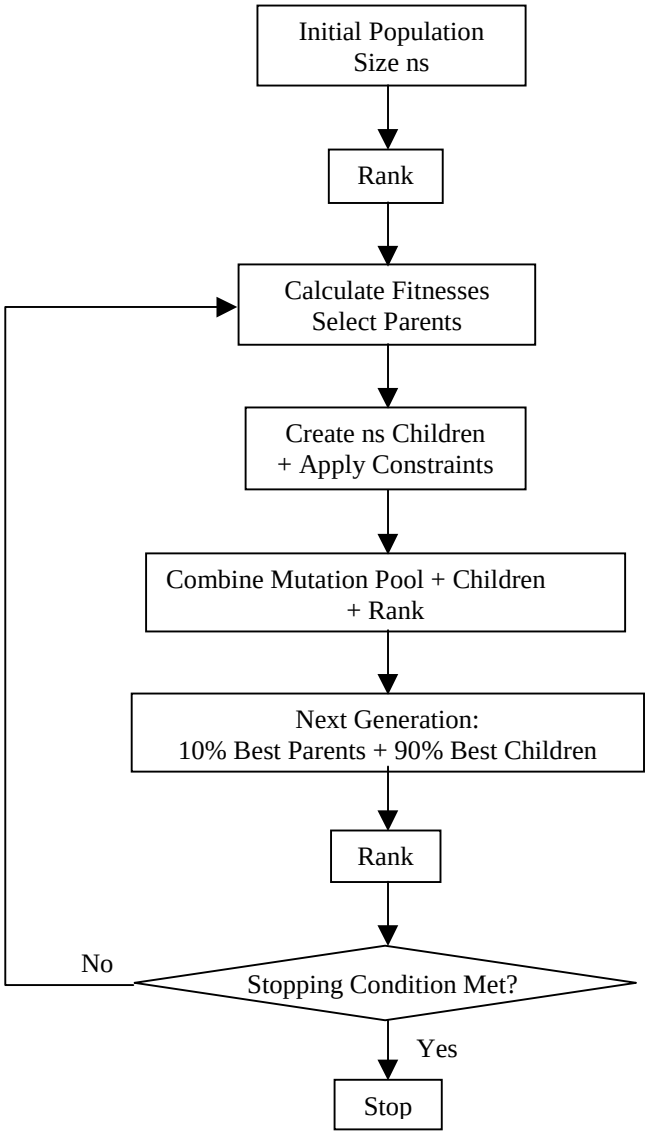

Figure 4.4 Simplified flowchart of GA_3.

the current research (Sections 5.1.2, 5.2.1, 5.2.2 and Chapter 6), the values used for the setting of the genetic parameters (p_t, p_c, p_{mj}, p_{mc} and p_r) were determined from a performance analysis described in Section 4.4. The major enhancements with the EEGA came from the use of:

1. binary tournament selection (see Paragraph *selection* in Section 4.2.4) which helps prevent premature convergence (Goldberg, 1989). An elitist scheme was actually implemented in which each chromosome of the top half of the current ranked population competes with a second chromosome randomly chosen from the entire population (and which cannot be a duplicate of the first chromosome). The chromosome with the higher fitness value is inserted into the mating pool with a probability p_t set to 0.9 (in 10% of the cases, the parent selected is the less fit).
2. an arithmetic crossover (Doyle, 1994) well suited for real encoding and which allows for the creation of new genes even outside the initial parameter ranges. Two children C_1 and C_2 are created per pair of parents P_1 and P_2 with a probability p_c taken as 0.9 (10% of the parents are cloned) using: $C_1 = \left(\frac{P_1 + P_2}{2}\right) + \left|P_1 - P_2\right| \times R, \quad C_2 = \left(\frac{P_1 + P_2}{2}\right) - \left|P_1 - P_2\right| \times R,$ where R is a random number uniformly distributed between 0 and 1.
3. both the jump mutation and the creep variant with probabilities $p_{mj}=1/n_s$ and $p_{mc}= p_{mj}/2$, respectively, where n_s is the population size. The chromosome before mutation is copied onto a "mutation pool" and when the elitist replacement is applied (see below), the mutation pool is mixed with the resulting children pool. This means that good gene information is not lost by applying mutation.
4. an elitist generational replacement with a probability $p_r=0.9$, in which 10% of the top ranked parent population was kept into the next generation while 90% were replaced with the 90% best created chromosomes from the combined pool as described above.
5. a convergence criterion based on a small percentage change (1%) in both all gene values and the objective function value of the best (so far) chromosome (recall that the objective function is the optimality criterion, to be maximized, when performing experimental design optimization, and the least-squares error, to be minimized, when performing parameter estimation). The stopping condition is to first, execute *MING* generations without checking the convergence criterion. Next, this latter is checked at the end of each generation. If it is met during *LASTCRITERG* generations, then the run is stopped; if not, then at most *LASTG* generations are executed. Note that if the convergence criterion is

met for a number of generations less than *LASTCRITERG* and then the best-so-far chromosome changes, then the generation counter for the convergence criterion is reset.

In addition to these five points that are related to genetic operations, some improvements were made by using two types of nondimensionalization for the chromosomes. When the parameter range to investigate [parmin-parmax] (in which the initial population is defined) was less or equal than 2 orders of magnitude, e.g. $\frac{parmax}{parmin} \leq 100$, then a linear nondimensionalization was used; otherwise, a logarithmic nondimensionalization was applied, allowing then for large ranges to be scanned. Regardless of which type was used, the chromosomes were defined between zero and unity. In terms of the population size, a formula for binary encoding (Carroll, 1996a,b) was thought to be applied for real representation. The ideal population size was taken to be the product between the number of parameters to be determined and the average number that the parameters could take. Therefore, with a nondimensionalization between zero and unity, considering the case where the parameters could take 100 values in that range, the ideal population size was defined as $n_s = 100 \times n_p$.

A last improvement in developing the GA_3 is related to an important aspect of the optimization (or estimation) process. This aspect deals with applying knowledge-based control mechanisms to improve the solution. Constraints are a convenient means of incorporating domain knowledge as much as possible. In the GA_3, such incorporation was realized in two ways. First, into the fitness function (which is simply the objective function) by assigning penalties for chromosomes whose raw fitnesses were known to be infeasible. Those penalties made the chromosome be rejected when the elitism operator was applied. Second, constraints were also applied directly on the genes so that the search focused on the prescribed parameter ranges (note that these ranges were usually quite large for the first run). In this second way, any created gene that was lower than zero or higher than unity (which could happen with the use of the arithmetic crossover) were redefined as zero and unity, respectively. Analyses of the final population would indicate whether the prescribed ranges were adequate or not (for instance, if the genes were concentrated around zero or unity, then the prescribed ranges were inadequate).

Finally, note that in the GA_3 scheme, several EEGA features were removed, namely:

- the initial random search which resulted in an initial elitist population but was too computationally costly;
- the dangerous (because concentrated the search on local optima) procedure that updated the parameter ranges, and
- the procedure that eliminated the twins as no twins could be generated with the new crossover (this also had the effect of removing the procedure that inserted random chromosomes to replace the twins eliminated).

Also, note that, like with the EEGA, when the GA_3 was used as an estimation procedure, the output for a particular experimental data set included the means of each gene (thermophysical parameter) and the approximate 95% confidence intervals [Eq. (3.17)] representing the ranges of values in which the actual properties lay for that particular experiment.

- **Discussion**

With these attributes, the GA_3 algorithm was expected to show a better balance between exploitation (of the current population) and exploration (of new good solutions) than the EEGA. One very important point is that the number of evaluations performed with the GA_3, which can be approximated by $f_{eval} = n_s \times \left(n_g + 1\right)$, is, for the same population size n_s and number of generations n_g, much lower than with the EEGA. Therefore, in terms of computation cost, the GA_3 was a definitive improvement over the EEGA.

The results obtained using the GA_3 (Sections 5.1.2, 5.2.1, 5.2.2 and Chapter 6) showed that this algorithm performed very well, especially as far as not directing the solution to local optima. However, the weakness of the convergence criterion was highlighted in estimation applications in which the sensitivity of the measured quantity to some parameters was very small. Therefore, one of the recommendations of this work (Chapter 7) concerns the definition of a more suitable convergence criterion, in direct relation with the sensitivity of the measured quantity to the genes (parameters).

An issue when developing the GA_3 was the need for flexibility and adaptability so that the algorithm could handle both the Experimental Design Optimization (EDO) and

Simultaneous Parameter Estimation (SPE) of a problem since the direct solution is unchanged. Therefore, some key constants (flags) were defined so that by changing their default values and defining the appropriate genes (parameters), the GA_3 would perform either EDO (according to *D*-, *E*- or *A*-optimality by setting the appropriate flag) or SPE. The idea behind using such judicious default values (that are all specified in a default subroutine) was taken from the structure of the excellent program CONDUCT developed by Patankar (1991). Based on the GA_3 genetic features, and the flexibility for both EDO and SPE, two algorithm versions, GAMAIN and GACONDUCT were developed. Both versions follow the general structure of CONDUCT, e.g. they consist of an adaptation and an invariant part. The invariant part contains the general calculation scheme that is common to all possible EDO/SPE applications within the overall restrictions of the respective version used. The adaptation part provides the problem specification. The GAMAIN version was written for the analysis of problems for which a mathematical direct solution is to be provided by the user. For heat transfer problems for which an analytical solution does not exist, the GACONDUCT version was then developed by combining the general features of the GA_3 with those of an extension of the program CONDUCT, which is based on a control-volume-based finite difference numerical method. This extension involves modifications made by Dr. D. J. Nelson[1], which allow for the study of orthotropic properties in rectangular geometry (for instance k_x and k_y). Note that by benefiting from the possibilities of the program CONDUCT, the use of GACONDUCT allows for any EDO/SPE applications that deal with the computation of conduction and duct flow heat transfer in two-dimensional rectangular or cylindrical geometry.

Multiple comments are implemented throughout both versions and explain the meaning and the possible setting (depending on the problem to be solved) of the different key flags. Appendices B and C provide the listings (Fortran files) of GAMAIN.FOR and GACOMMON_MAIN.FOR, and GACONDUCT.FOR and GACOMMON_CONDUCT.FOR, respectively.

[1] Professor of Mechanical Engineering at Virginia Tech.

4.4 Performance Analysis of GAMAIN

To illustrate the performance of the GA_3 and to determine the "optimal" setting of the genetic parameters (p_t, p_c, p_{mj}, p_{mc}, and p_r), a mathematical test function was optimized using GAMAIN. The following provides a brief description of this function along with the results for the optimal setting.

4.4.1 Description of the Mathematical Test Function

The expression of the mathematical function **f6** optimized is shown in Eq. (4.1). This function was used by Schaffer et al. (1989) and Davis (1991) for the evaluation of different GAs.

$$f6(x,y) = 0.5 - \frac{\left[\sin\sqrt{x^2+y^2}\right]^2 - 0.5}{\left[1.0 + 0.001\times\left(x^2+y^2\right)\right]^2}, \quad x,y \in [-100,100] \tag{4.1}$$

This function is symmetric in x and y. Note that the expression for **f6** could have been simplified using the norm $r = \sqrt{x^2+y^2}$, but then, the complexity of this function would have disappeared. Figure 4.5 illustrates the distribution of this function with y being held constant at its optimal point while x ranges from –100 to 100 (the same graph would be obtained if x and y were switched). The goal is to optimize **f6**, e.g. to find values of x and y which produce the greatest possible value for **f6**. This function has several features that make it an interesting test case:

1. **f6** has a single global optimum (which is **f6(*x*=0,*y*=0) = 1**);
2. **f6** shows strong oscillations with increased magnitudes until the global optimum is reached; this is often called multimodality;
3. the global region occupies a tiny fraction of the total area

From this, one anticipates the output from the application of a gradient-based method to become "stuck" on a local hill.

4.4.2 Results

The listing of the adapt subroutine GADAVISF6.FOR (that works with the program GAMAIN given in Appendix A) is provided in Appendix D. Only the results of the analysis of the effects of the genetic parameter settings are reported here. The optimal setting for the genetic parameters investigated is shown in Table 4.1. This setting was found to be superior to any others as it allowed the global optimum of the function **f6** to be found with a 100% probability (on the basis of 20 runs).

Table 4.1 Genetic parameter optimal setting (n_p=2).

n_s	p_t	p_c	p_{mj}	p_{mc}	p_r	*MING* [(1)]	*LASTCRITERG* [(2)]
200 $=100n_p$	0.9	0.9	0.005 $=1/n_s$	0.0025 $=p_{mc}/2$	0.9	20	20

[(1)] initial number of generations that must be performed without checking the convergence criterion.
[(2)] number of generations during which the convergence criterion must be satisfied.

Figure 4.6 shows a typical increase of both the fitness (function **f6**) of the best individual and the average fitness of the population, while Fig. 4.7 illustrates the population evolution from the initial to the final state.

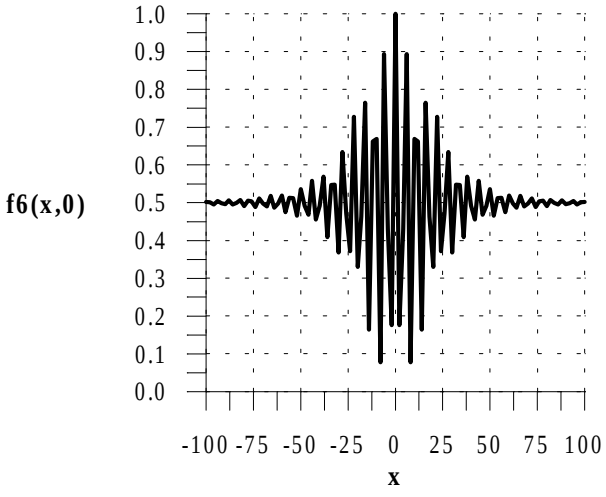

Figure 4.5 Function f6 vs. *x* with *y* set to 0.

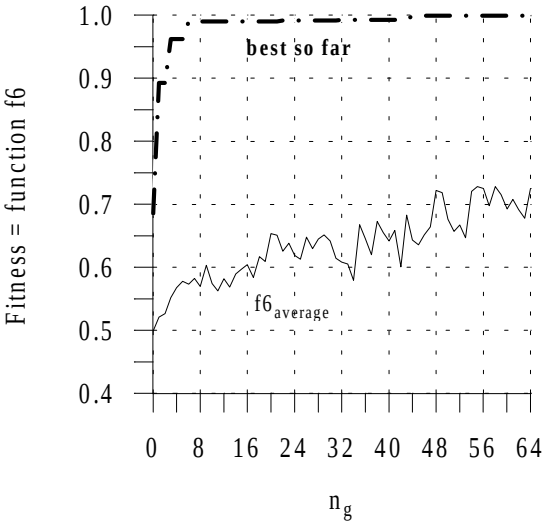

Figure 4.6 Fitness evolution vs. n_g.

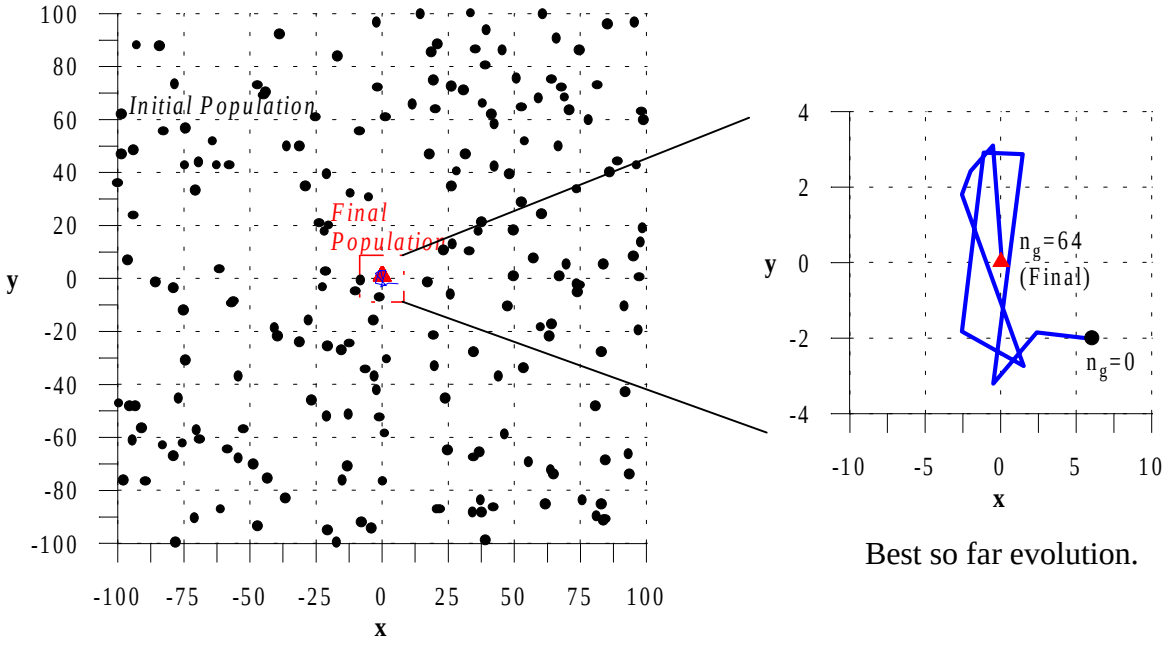

Figure 4.7 Population evolution (initial to final generation).

Because settings of genetic parameters can be a very difficult and time intensive task, the optimal setting found for the optimization of the function **f6** was used subsequently (except for n_s, *MING*, and *LASTCRITERG* that were problem dependent). Note that this setting was probably not the best in all problems treated subsequently; however Davis has reported that robust settings work well across a variety of problems.