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Modeling and optimization of multi-component materials selection and sizing problem

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Abstract

Most of the research on materials selection has been characterized by a basic approach to the problem, isolating material choice from the other design variables, and focusing on single components. Instead, a complete approach aimed at optimizing material selection cannot be set aside from component sizing, and the analysis of constraints between components, that characterize the sub-assemblies or the whole system, and can influence the material choice itself. In this paper, a structured method to approach the simultaneous materials selection and sizing optimization of multi-component assemblies is proposed. It is based on a modeling of the problem, fully generalized in its formalization, so as to be applicable to the various cases, and formulated in order to take into account the systemic vision that must have the optimal choice in a multi-component perspective, and its close connection with the sizing of geometric variables, to effectively meet the required performances. In this regard, an efficiency criterion, which provides for the choice of material and variables sizing gauged on real needs, is also introduced. After presenting the framework and formalization of the method, the problem of searching for the best solution has been discussed. With regard to this, a genetic algorithm has been specifically developed according to the peculiarities of the generalized formulation, with the aim of enhancing the heuristic potential of the concurrent material choice and sizing approach in multi-component environment, in the search for the optimal solution. The application to a sub-system of a widely used plant device is reported in detail, so that use and capacity of the structured method are detailed and discussed.

Keywords

Materials selection, component sizing, multi-component environment, efficiency criterion, genetic algorithm

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Introduction

The great variety of materials available for engineering applications extends the design possibilities, but combined with the complexity of the set of requirements that influence the choice of the most appropriate materials involves a problem of multi-criteria decision analysis and optimization of considerable difficulty.

Basic materials selection activities have been identified in formulating design requirements and materials specifications, making a set of candidate materials by screening on primary rigid requirements, comparing and ranking them to identify those that have the highest potential, refining the final choice on top-ranked solutions.[1–4] A wide variety of quantitative models have been developed to allow systematic evaluations in these basic steps of the selection process.[5–12]

Used with the support of the simplest multi-objective analysis tools,[5,13] or combined with more sophisticated multi-criteria decision making techniques,[14–19] the analytical and graphic tools provided by these methods allow a rational selection of the materials more suitable to the required use. They all focus the intervention on components considered singly, without taking into account the systemic context for which each of them is intended, and isolating the choice of the material from the definition of the other design variables, delegating to other interventions the sizing of significant geometric variables.

To overcome the basic single-component approach that has characterized most of the research conducted

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on materials selection, the importance of integrating material choice and optimal dimensioning, as been set off.[20] The search for optimal cross-section shape in this field has been a first example.[21,22] The interactions between material properties and component geometrical properties (shape and size) has been discussed.[23] Starting from a pre-selection of ideal candidate materials, mathematical formulations for structural optimization,[24] or simplified models for calculating and comparing the optimal solutions for selected ideal materials,[25] have been proposed. Other studies has been dedicated to integrated selection of material and geometric variables with regard to specific engineering problems, such as truss structure optimization,[26,27] automotive body assembly,[28] and gear design.[29] An analysis of the optimization problem, with particular regard to the mathematical properties of the solution domain has been also presented.[30]

From this general overview on the approach to materials selection problem, the following conclusions can be drawn:

- Most of the research conducted on materials selection has been characterized by a simplified approach to the problem, isolating the choice of the material from the definition of the other design variables;
- Even when some form of combination between the choice of materials and the dimensional optimization of components has been introduced, the integration is not completely concurrent, and the proposed models are not generalized;
- The problem is treated by excluding the systemic point of view, focusing the intervention on the single components, and thus decoupling the overall design problem into sub-problems on components considered one by one.

Starting from these premises, an approach to the simultaneous choice of material and sizing of multi-component assemblies, based on a generalized modeling of the problem, is proposed. The approach also takes into account the systemic dimension that must have the optimal choice of material for each component. The modeling and statement of the problem are characterized by the following peculiarities:

- They have been developed in generalized form, in order to outline a basic instrument, applicable to the diversified specificities of the materials choice problems;
- For each component that constitutes the assembly, the choice of material with the sizing are combined, by defining simultaneously the free geometric variables of the problem;
- While operating at the level of the single component, the constraints to be imposed on the distribution of materials in a multi-component perspective are taken into account, that are the constraints deriving from the various types of interaction between the components of the whole system.

The problem of multi-criteria analysis and optimization, that is complex already in the simple choice of the best material for a single component, becomes much more complex when the design effort is extended to simultaneous materials distribution and components sizing in multi-component assemblies. As a consequence, the management of this high level of complexity could go to deter the effectiveness of design, losing sight of the aspects related to the adequacy of design choices. For this reason, as a further feature of the proposed model, the distribution of the materials among the components of the assemblies, and the sizing of the components, will be guided by applying an efficiency principle, which provides for the choice of material and sizing gauged on the real performance needs of each component, avoiding oversizing and/or resorting to materials excessively performing for the required use.

The underlined complexity of the problem suggest also the use of evolutionary optimization tools, as already proposed by other authors to solve more conventionally formulated problem of multi-objective materials choice.[28,30–33] In particular, it was considered that the use of a genetic algorithm could allow to overcome the criticality of other tools, operating directly on an objective function which interprets the different aspects of the whole problem, and investigating both the domain of discretized variables, which identify the choice of materials, and the complete ranges of continuous values of the geometric parameters to be sized. With these premises, a genetic algorithm has been specifically developed in the MATLAB environment. It has been structured and characterized according to the peculiarities of the generalized formulation of the concurrent material choice and sizing problem, extended to multi-component systems, with the aim of enhancing its heuristic potential in the search for the optimal solution.

After presenting the formalization and modeling of the problem and the characteristics of the algorithm developed, an application to a sub-system of a widely used plant device will be reported in detail.

Basic framework of the methodological approach

In the design process, system and component design represent the two levels through which, based on the concept outlined in the previous design phases, the requirements take shape in a concrete solution.[4,34] Materials selection, although it can be applied preliminarily in the previous phase of concept design,[35,36] assumes a decisive role precisely at these levels of the design process.

Schematized in Figure 1, the materials selection procedure that is proposed here is integrated into

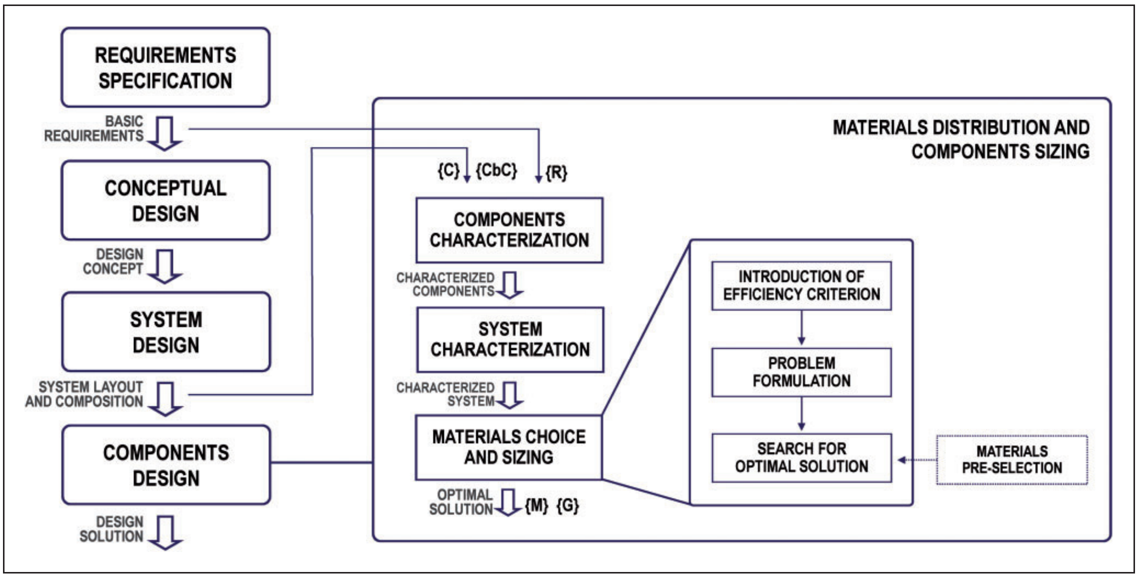

Figure 1. Basic framework of the approach to the problem and structure of the method.

the design development process, and draws information from the specification of the requirements and from the development of the design at the system level.

The procedure is articulated according to the preliminary steps of components and system characterization, aimed at defining the requirements, objectives, constraints, and variables related to each component and to the whole system; the core step of materials choice and components sizing, in which the efficiency criterion is introduced, the complete problem is formulated, and the search for optimal solution is performed.

Analysis of requirements and system composition

The process of materials selection and sizing of the components, structured according the procedure outlined in Figure 1, is based on the specification of the design requirements, from which it is possible to derive the requirements to be associated with each component, and on information specified at system design level, which defines the layout of the technical system, and the subdivision into sub-assemblies and components.

In formulating the design problem, for the sake of brevity the generic term ''system'' will be used to indicate a multi-component assembly, be it one of the subassemblies in which the technical system can be divided, or the whole technical system, if it is not subdivided into sub-systems.

Specification of requirements

The requirements that express the objectives of the problem (optimizing masses, costs, or other performance functions), and the constraints within which these objectives should be pursued (loads to resist, thermal flows to be transmitted, etc.), will be attributed to the components, and translated into objective functions and constraint equations on requirements. The latter, together with constraints on geometric parameters and on material properties, will guide the choice of material and the dimensioning of free variables in optimizing functions that express the objectives of the problem.

The requirements that express the objective functions are:

- Functional requirements: They express the functional properties required to the system and its components that are derived from the primary needs from which the design originates.
- Requirements related to physical properties of components and the system: The overall dimensions of the system as a whole, and/or some of its components, and the weight, also referred to the whole system or to its specific components, are among the most common requirements of this type.
- Manufacturability and cost-effectiveness requirements: They interpret the possibility to realize components and the system in the most efficient and economic way, and are generally quantified by cost functions.

The requirements that express the conditions under which the objective functions must be performer can be:

- Requirements related to physical phenomena: They concern the behavior of components and the system with respect to physical phenomena of

various types, due to the operating conditions (mechanical, thermal, electric, magnetic, optical). Among these, the requirements related to mechanical phenomena (e.g. resistance to static loads, to fatigue and fracture mechanisms) are very common in engineering applications, since they guarantee the stability of the structural behavior of the system.
- Requirements regarding the environmental conditions: They concern the behavior of components and the system with respect to the environmental conditions under which the system performs its functions. Among these requirements, very common are the resistance to thermal stress, corrosion, oxidation, attack of acids and other agents.

The first class of requirements is often referable to functions that express volumes, masses, costs, to be minimized, but in general terms it can be represented by a range of functions as large as the possible fields of application of the system. The second class of requirements, defined above in qualitative terms, express functional constraint conditions, and are defined quantitatively by the "stresses", in generalized meaning (using an analogy with the phenomena of structural resistance), which the components or the whole system must endure: mechanical loads, impact or vibration energy, thermal loads, and any other physical entity quantifying conditions that fall on the system or single components (or "stress" them).

The former class expresses the set of requirements to be optimized $\{R_{opt}\}$, the latter expresses the set of requirements due to functional constraints $\{R_{constr}\}$. In the formulation of the design problem for the system and its components, $\{R_{opt}\}$ and $\{R_{constr}\}$ translate into objective functions and constraint equations on the requirements, respectively, and together constitute the set of basic requirements $\{R\}$.

Formulation of system composition

At the end of system design, the architecture and layout, with subsystems and components are defined, and the correlations that link them together are outlined. The obtained system composition is represented by:

- The set of components $\{C\}$, that collects the n_c components constituting the system $\{C_1,\ldots, C_i,\ldots, C_{nc}\}$;
- The set of constraints between components in the whole system $\{CbC\}$, that describe the network of correlations between components in the design process.

The components are correlated in the design process means they are correlated in terms of requirements, functionalities, geometric parameters, and/or materials.

Materials distribution and components sizing problem formalization

The whole set of constraints, consisting of the constraints on the requirements included in the set $\{R_{constr}\}$ (section "Specification of requirements") and the constraints between the components of the set $\{CbC\}$ (section "Formulation of system composition"), expresses the conditions that regulate the modalities according to which the functions are performed, and are fundamental to guarantee the required performance (e.g. constraints on resistance to loads, on admissible deformations, etc.), in compliance with the necessary restrictions (constraints on geometric parameters and shapes, constraints on service conditions, such as temperature range and other environmental conditions). The objectives of the problem, expressing the requirements gathered in the set $\{R_{opt}\}$ (section "Specification of requirements"), quantify the properties of the components or the system to be optimized (lightness, economy, safety, even combined), and allow to qualify a solution as optimal with respect to the other ones.

The materials distribution and components sizing procedure (Figure 1) elaborates all this information in three phases: components characterization, which consists of defining and formalizing the requirements, objectives, constraints, and variables related to each component; system characterization, which extends the same formalization at system level; materials choice and components sizing, in which the characterization of each component and of the system converge in the formalization of the problem of optimal choice of materials and sizing of the components, and in which the most suitable tools can be applied to search for the solution of the problem.

Components characterization

The set of requirements $\{R\}$, previously defined by the requirements specification phase (section "Specification of requirements"), is translated into requirements on the components $\{RoC\}$ that specify for each ith component C_i the set of requirements $\{RoC\}_i$ concerning it. Defining the set $\{RoC\}_i$, for each component, the design problem consists in defining the geometric parameters G_i, which specify the shape and sizes, and its material M_i, and can be formulated identifying objectives, constraints, and variables.

The objectives of the design problem express the requirements on the components to be optimized $\{RoC_{opt}\}$. In general, with regard to the ith generic component, each objective that expresses the requirements on the component $\{RoC_{opt}\}_i$ can be formulated by an objective or performance function PF, to be minimized or maximized, in the generalized form

$$PF = f_1[G_F, G_V, M_T P_R, (RoC_{constr})] \tag{1}$$

that is a function of groupings of variables: specifications on geometry G_F and G_V (fixed and variable geometric parameters of the component); properties of material M_TP_R; and in the most general form, requirements on the component, to be constrained RoC_{constr}. With regard to the primary objectives in design, which consist of limiting the volume, weight, and cost of the final solution, they are not directly dependent on requirements to be constrained RoC_{constr}. This is the meaning of the term RoC_{constr} in brackets in equation (1).

The minimization (or maximization) of each PF can be subject to different types of constraints:

- CoR – Constraints on requirements to be constrained RoC_{constr};
- CoG – Constraints on geometric parameters G_F and G_V;
- CoM – Constraints on material properties M_TP_R.

In general terms, with regard to a generic component, the constraints on each requirement to be constrained CoR can be expressed by a constraint equation in the form

$$S \leqslant f_2[G_F, G_V, M_TP_R, (O_TC_OP_R)] \quad (2)$$

Using the analogy with phenomena of structural resistance introduced before (section "Specification of requirements"), the first term S stands for the "generalized stress" to which the component must resist (that quantifies a requirement of RoC_{constr} type), the second term stands for the "generalized resistance" of component to this stress. Therefore, constraint equations (2) can be also formulated in the form of constraint ratio CR, as the ratio between component resistance and the stress to which it is subjected, that should be higher than 1

$$CR = \frac{f_2[G_F, G_V, M_TP_R, (O_TC_OP_R)]}{S} =$$

$$= f_3[RoC_{constr}, G_F, G_V, M_TP_R, (O_TC_OP_R)] \geqslant 1 \quad (3)$$

Constraints CoG on geometric parameters G_V and G_F of the component can be expressed as constraint limits, and fixed value required, respectively

$$G_V \leqslant\geqslant G_{V\lim} \quad G_F \equiv G_{F\mathrm{req}} \quad (4)$$

Similarly, constraints CoM on the properties of the material M_TP_R can be expressed as constraint limits in the form

$$M_TP_R \leqslant\geqslant M_TP_{R\lim} \quad M_TP_R \equiv M_TP_{R\mathrm{req}} \quad (5)$$

The conditions of type (5) express those that are the primary constraints on the choice of materials, which allow the screening on the set of materials available for the solution of the design problem. These primary constraints are those that interpret the essential requisites on material properties that the design must satisfy, and which translate into two types of conditions to be imposed:

- Limit conditions: It is the case in which a requirement results in a minimum or maximum limit to be imposed on one or more properties of the material; the limits can be quantitative or qualitative, depending on whether it is imposed on a quantifiable property of the material, or on a nonquantifiable property (in this second case, the property and its limits are expressed in a qualitative form, such as low–medium–high). In generalized form, this type of condition is expressed by the first condition of type (5).
- Boolean-type conditions: In this case, the requirement is expressed in Boolean terms (the property of the material does/does not satisfy the requirement); this is the case, for example, of Boolean constraints on the processability (compatibility between the material and the processes to manufacture the component). In a generalized form, this type of condition is expressed by the second form of the constraint equations (5).

With all these premises, the basic design problem for the ith component C_i can be formulated as follows: define the geometric parameters G_i and the material M_i that optimize (or balance) the set $\{PF\}_i$ of type (1) objective functions, while respecting the whole set of type (2) or (3) constraints on requirements $\{CoR\}_i$, type (4) constraints on geometric parameters $\{CoG\}_i$, and type (5) constraints on material properties $\{CoM\}_i$.

System characterization

The previous formalization of objectives, constraints, and variables of the design problem refers to the case where the generic component is independent of the other components in the system. If the generic component C_i depends on other system components, the set $\{CbC\}_i$, which is a subset of the set of constraints between components in the whole system $\{CbC\}$, and collects the constraints between ith component C_i and other components of the system, must be met. In the simplest cases, these constraints are expressed directly or indirectly in equations (1), (2), (4), (5) of one or more single components:

- The most common constraints between components are on geometric parameters G_V and/or G_F. In this case, the constraint limits $G_{V\ lim}$ and/or $G_{F req}$ in equation (4) depend on the geometric type properties of other components. As a consequence, geometric parameters G_V and/or G_F in equations (1) and (2) are constrained by properties of other components $O_T C_O P_R$.

- Another common potential constraint between components could take place on materials (e.g. because of incompatible materials). In this case, some constraints on materials properties in equation (5) depend on the properties of other components, related to their material. As a consequence, material properties $M_T P_R$ in equations (1) and (2) are constrained by the properties of other components $O_T C_O P_R$.
- If a component is related to another component at functional level, in equation (2) the generalized function f_2 depend on the properties of the other component also. This is the meaning of the term $O_T C_O P_R$ in brackets. The same observation can be repeated for the generalized formulation (3) of the constraint ratio CR. This case of constraints between components includes the condition of same requirements shared among components.

Apart from these specific cases, in general terms, the constraints between components of the set $\{CbC\}$, which is referred to the whole system, are not attributable to the single components, but instead to different combinations of them, and must be expressed by means of constraint equations apart, whose generalized form is

$$f_4[G_{F\mathrm{i}}, G_{V\mathrm{i}}, M_T P_{R\mathrm{i}}, (RoC_{constr\ \mathrm{i}})]_{i=1,\ldots,n_{c1}} \leqslant \geqslant \\ \leqslant \geqslant f_5\big[G_{F\mathrm{j}}, G_{V\mathrm{j}}, M_T P_{R\mathrm{j}}, (RoC_{constr\ \mathrm{j}})\big]_{j=1,\ldots,n_{c2}} \tag{6}$$

where f_4 is a function of the groupings of variables $G_{F\,i}$, $G_{V\,i}$, $M_T P_{R\,i}$, and if the case arises, requirements to be constrained $RoC_{constr\ i}$, of a part (in number equal to n_{c1}) of the n_c components constituting the system; the second term f_5 is a function of the groupings of variables $G_{F\,j}$, $G_{V\,j}$, $M_T P_{R\,j}$, and if the case arises, requirements to be constrained $RoC_{constr\ j}$, of another part (in number equal to n_{c2}) of the n_c components constituting the system.

Efficient materials choice and components sizing

As already anticipated before, a further feature of the proposed approach is to allow the search for the solution to be guided by applying an efficiency principle, which provides for the choice of material and the sizing gauged on the real performance needs.[37] This principle translates into a further type of performance equation, which will be referred to as the efficiency function EF

$$EF = \frac{1}{CR} = f_7[RoC_{constr}, G_F, G_V, M_T P_R, (O_T C_O P_R)] \tag{7}$$

With CR $\geqslant 1$, the EF efficiency function expressed by equation (7) takes values in the interval [0, 1]. If maximized, EF ensures that the constraint on requirement CoR of type (2) is respected as efficiently as possible, i.e. in such a way that the component's resistance overcomes the stress to which the component is subjected, minimizing the gap between the two factors. This means weighting the choice of the material and the free geometric variables in order to guarantee the constraint on the requirement, but also avoiding to choose materials that are excessively and unnecessarily performing with respect to the requirement, and without oversizing the geometric variables to excess.

The efficiency principle implemented in this way, as well as avoiding unnecessary economic costs, responds to more general economic criteria, which look to a responsible use of materials, both from a quantitative and qualitative point of view, and translate into efficient design choices, i.e. such as to guarantee functionality and required performance levels, by mean of the minimum effort.

Complete formalization of materials choice and components sizing problem

In the last step of the procedure, the characterizations of individual components (section "Components characterization") and the system (section "System characterization"), and the introduction of the efficiency criterion (section "Efficient materials choice and components sizing"), converge in the formalization of the problem of optimal materials choice and components sizing, for a multi-component system that ultimately requires the following:

- Distribution of the $\{RoC\}$ requirements among the $\{C\}$ components of the system;
- Formulation of the performance functions $\{PF\}$ for each component (to be minimized or maximized), expressed by the equations of type (1);
- Formulation of the constraints on the requirements $\{CoR\}$ for each component, according to the equation of type (2), and in the form of the constraint ratio CR (3);
- Formulation of the efficiency functions $\{EF\}$ (to be maximized), in the form (7);
- Definition of the set of constraints on geometric parameters $\{CoG\}$, in the form (4)
- Definition of the set of constraints on the materials $\{CoM\}$, in the form (5)
- Definition of the set of all the constraints between components $\{CbC\}$ in the whole system, in the form (6), or directly expressed in equations (2), (4), and (5).

Therefore, the problem of optimal materials choice and components sizing, for a system constituted by the set $\{C\}$ of n_c components, can be formulated as follows: define the geometric parameters $\{G\}$ and the materials $\{M\}$ of the whole set $\{C\}$ of components that optimize (or balance) the set $\{PF\}$ of type (1) objective functions, and the set $\{EF\}$ of type (7) efficiency functions (to be considered as further objective functions), while respecting the whole set of type (2) or (3) constraints on requirements $\{CoR\}$, the type (4) constraints on geometric parameters $\{CoG\}$, and the type (5) constraints on material properties $\{CoM\}$ for all the components of the set $\{C\}$, and the set $\{CbC\}$ of all constraints between components in the whole system, of type (6), or directly expressed in equations (2), (4), and (5).

The objective functions $\{PF\}$ and $\{EF\}$ can be collected in one overall function using simple multi-objective analysis models, which allow to define single functions as a weighed sum of normalized objective functions, even inhomogeneous, indifferently to be maximized or minimized.[5] The introduction of weight coefficients allows to qualify the overall function, depending on the distribution of the values to be attributed to these coefficients. The single objective function that is obtained in this way will be of the type

$$\Theta = \sum_{i=1}^{n_{PF}} \alpha_i \cdot \overline{PF}_i + \sum_{j=1}^{n_{EF}} \alpha_j \cdot \overline{EF}_j \tag{8}$$

where $\overline{PF}_i$, $\overline{EF}_j$, represent the normalized values of the objective functions $\{PF\}$, $\{EF\}$; n_{PF}, n_{EF}, represent the corresponding numbers of these functions, to be taken into consideration in the specific case; α_i, α_j, are the weight coefficients $(\Sigma\alpha_i + \Sigma\alpha_j = 1)$.

Functions $\{PF\}$ and $\{EF\}$ can be normalized with respect to the whole set of potential solutions, so that regardless of whether they should be maximized or minimized, the corresponding normalized values must always be minimized. In this way, for each potential solution it is possible to calculate the value of the single objective function Θ, so as to obtain the ranking of the potential solutions, and identify the optimal solution, that is the one that minimizes Θ.

The proposed formalization of the problem, and its generalized modeling, can be used to apply in a systematic way the analytical and graphic tools provided by other well-known materials selection methods.[5–12] It can be useful to systematize and manage multiple variables-constraints types of selection problem, such as overconstrained problems,[4] and it is suitable to be integrated with multi-objective analysis tools and multi-criteria decision-making techniques commonly used in the field.[19] In these terms, what is proposed provides a methodological framework, and the complete modeling, for the extension of previous materials selection techniques, so to assist a rational distribution of the materials and sizing in multi-component system design.

Search for the optimal solution

Having obtained a single function to be optimized (8), the problem of finding the best solution, while respecting all the constraints, must be addressed. An exhaustive analysis of all potential solutions would require the definition of a reasonably limited set of potential materials to be distributed among the components, and discretized ranges of potential values for the geometric parameters to be sized. In this case, a preliminary pre-selection of the materials is necessary (this could be one of the meanings of the box in dashed line, in the diagram of Figure 1), to limit the search domain on which to apply exhaustive procedures. The pre-selection could be based on the designer's experience and best practice criteria. Structured methods for product examples analysis could be also used, in order to increase in a reasoned manner the number of alternative materials to be analyzed.[38] However, this type of approach, as is evident, can be used in the case of systems consisting of a very limited number of components. Furthermore, it does not allow a real optimization of the selection and sizing problem, which is reduced to a classification of potential solutions that are combinations of discretized geometric parameters and pre-selected materials.

The different types of variables involved in the real problem of distribution of materials in the system and sizing of components (discretized variables, for the identification of materials, and continuous variables, for the sizing of components), and the formalization of the problem proposed here, suggest the recourse to a genetic optimization algorithm.[39] Particularly suitable for managing multi-objective optimization,[40] also on wide and nonunimodal search domains,[41] this type of optimization tool allows to operate on continuous and discrete mixed variables, assuming as the objective function that expressed by (8), which interprets the different aspects of the whole problem, and avoiding to force the choice of materials within strongly limited search domains, which would affect the final result, so as to obtain a real simultaneous optimization of the choice of materials and the sizing of geometric parameters, even in compliance with the efficiency criterion. The appropriateness of the use this type of search algorithm in the specific case of shape, sizing, and material choice optimization problem has been confirmed from the mathematical point of view also, with particular regards to the effects of continuous and discrete mixed variables on continuity of the solution domain.[30]

Figure 2 shows the general framework of the algorithm specially developed, and implemented in MATLAB environment. It presupposes:

- the data restructuring for search procedure, whose purpose is to translate the results of requirements specification (section ''Specification of requirements''), analysis of system composition (section ''Formulation of system composition''), components and system characterizations (sections ''Components characterization'' and ''System

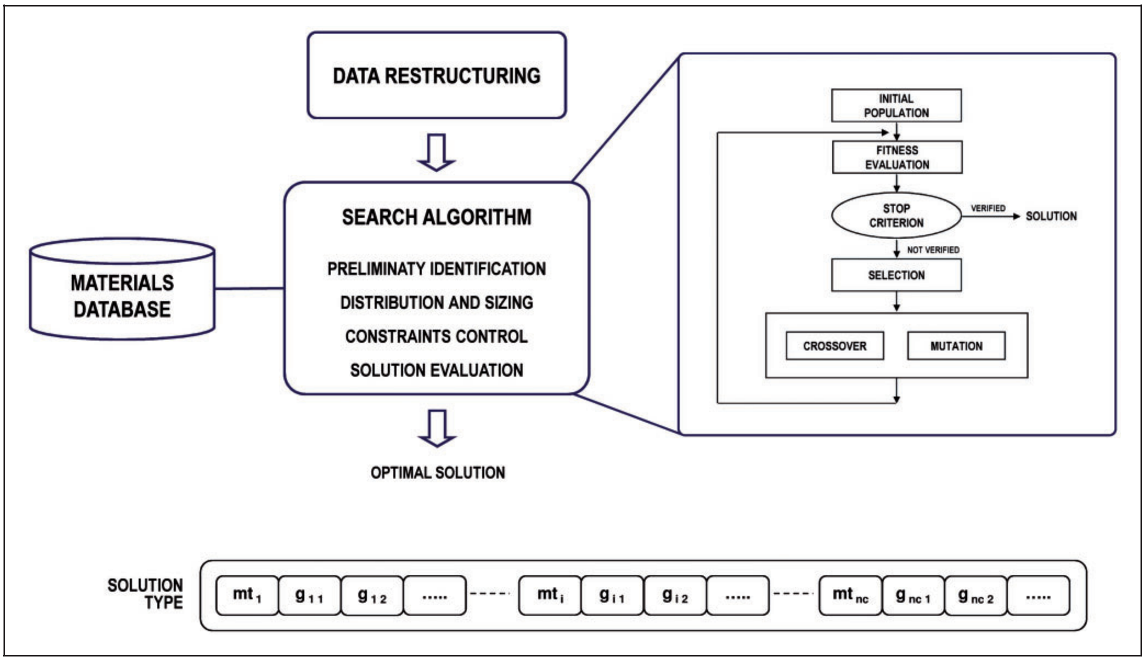

Figure 2. General scheme of the proposed algorithm.

characterization''), into mathematical terms suitable to be elaborated by the algorithm core;
- the compiling of materials database that allow the search algorithm to associate the properties that are involved in the formulation of the problem, to each potential material for the solution of the selection problem (the database module define each material by a characterization vector that collect the integer number expressing the material identification code M_{IC}, and the values of its properties involved in the formulation of the problem).

Getting information on material properties from the database module properly compiled, the algorithm core searches for the optimal solution through four main functionalities:

- Preliminary identification, that provides for the formalization of the solution type to be investigated and the definition of the objective function;
- Generation of potential solutions (materials distribution and components sizing for the whole system);
- Verification of constraint conditions and screening of potential solution;
- Evaluation of possible solutions and search for the optimal one.

Characteristics of the search algorithm

The structure of the genetic algorithm used is conventional, but for convenience it is shown in Figure 2. The algorithm operates on populations of individuals, to be understood as sets of points of the objective function domain. Each individual represents a potential solution, and is codified in a structure that recalls the chromosomal configuration (Figure 2).

As known, the algorithm first generates a random population. Subsequently, at every cycle of generation it selects individuals that satisfy all the constraints, based on their fitness (quantified by the value assumed by a fitness function), and applies genetic operators (crossover and mutation) on the individuals selected. The generation of a first random population expresses the need to explore the widest possible domain of potential solutions. On the other hand, it could limit the efficacy of the algorithm in converging towards valid solutions. For this reason, if in the first generation there are no valid individuals (i.e. solutions that respect the whole set of constraints, with a fitness of an acceptable level), the so called ''seeding'' can be operated, inserting a valid individual (seed) with a recognized good level of fitness in the population, to facilitate its evolution.

The algorithm has been developed and implemented in MATLAB environment. The coding of individuals and the definition of the fitness function will be treated in the following section. Its other features are as follows:

- Population size of 100 individuals;
- Steady-state population regeneration (part of the population survives from one generation to the next), with generation gap (population fraction replaced) of 0.9;
- Stochastic Universal Sampling selection, with elitist strategy (if the best individual should turn to be less fit than the champion from the preceding

generation, the latter is reinserted in the place of the less fit individual of the new generation);

- Single-point crossover with probability of application 0.7, and mutation with probability of application 0.7/length of the chromosome, as genetic operators;
- Stopping criterion based on fixed number of generations (50 was found to be a number suitable for convergence purposes).

Formalizations and functionalities of the search algorithm

The solution type of the algorithm has to be formulated to express the materials of system's components $\{M\}$ to be chosen, and the values of the variable geometric parameters of system's components $\{G_V\}$ to be sized. Its formalization consists in a sequence of subsets of variables, one subset for each one of the n_c components of the system (Figure 2). The first variable mt_i of each subset is the identification code M_{IC} (integer number) that identify the material of the ith component, according to the codification adopted in compiling the materials database. The subsequent variables of the subset g_{i1}, $g_{i2}, \ldots$, are the values of the geometric parameters G_V of the ith component to be sized (real numbers).

The generation of potential solutions (that means potential materials distribution and components sizing for the whole system) is intrinsic to the functioning of the genetic algorithm. Every individual in each generation (formalized by the vector of solution type in Figure 2) represents a potential solution. If a potential solution respects all the constraint conditions of the problem, expressed by equation (2) or (3), (4), (5), and (6), and therefore is a possible solution, then its fitness is evaluated. The fitness function is expressed by the objective function (8), to be calculated for the values of the variables constituting each potential solution by means of equation (1) and (7), using also the data collected in the material properties database.

The optimal solution will be found when the algorithm converges and stops. This solution is still expressed in the form of solution type in Figure 2, and consists of a sequence of subsets, each of them identifying a component of the system, and constituted by material identification code M_{IC} and values of geometric variables G_V to be sized. This represents the possible solution that defines materials distribution and component sizing, minimizing the objective function (8).

As is known, the characteristic of genetic algorithms is that of identifying solutions of local optimum. This implies, as a consequence, the possibility that the same algorithm, at the same search conditions, every time it runs, can identify different local optimal solutions. This, which may seem a limitation of the genetic approach to optimization, in reality turns out to be a particularly appropriate property in the solution of the materials selection problem. As a matter of fact, in the overwhelming majority of cases, for any application, more than one material is suitable, and the final choice is actually a good compromise to solve the problem.[42] In this regard, the precaution to avoid forcing the optimization towards the search for an univocal optimum, but rather to determine a set of effective solutions on which to make final qualitative evaluations, based on not-structured supporting information on materials (design guidelines, case studies and known applications, supplier information, standards and codes, etc.),[4,6] is always a sensible and well founded practice. Evidences of this aspect of the problem will be provided in the discussion on the reported case study.

Case study: Heat exchanger

The application of the proposed approach to materials choice and component sizing in the case of a subsystem of a shell-and-tube heat exchanger is reported. Taking into account the configuration shown in Figure 3, defined according the reference construction standard by Tubular Exchanger Manufacturers Association (TEMA),[43] and acquired the results of the thermodynamic dimensioning of the system,[44] the attention has been focused on the sub-system consisting of the main components of the central module: the shell, the tube bundle, and the tubesheets.

Components and system characterization

The preliminary analysis of the sub-system allowed to define the three basic components representing the design problem: shell (C_1), tube (C_2), tubesheet (C_3). The complete characterization of the components and the sub-system (according to section "Materials distribution and components sizing problem formalization") allowed to define objectives, requirements to be constrained, fixed and variable geometric parameters, for each component, as detailed in Tables 1 to 3, and the set of constraints between components, as detailed in Table 4. For each ith component, they have been defined:

- the sets requirements on components to be optimized $\{RoC_{opt}\}_i$, and to be constrained $\{RoC_{constr}\}_i$;
- the set of performance functions $\{PF\}_i$ to be optimized;
- the set of constraints on requirements $\{CoR\}_i$ to be satisfied, and efficiency functions $\{EF\}_i$ to be optimized;
- the set of constraints on geometric parameters $\{CoG\}_i$ and on material properties $\{CoM\}_i$, to be satisfied.

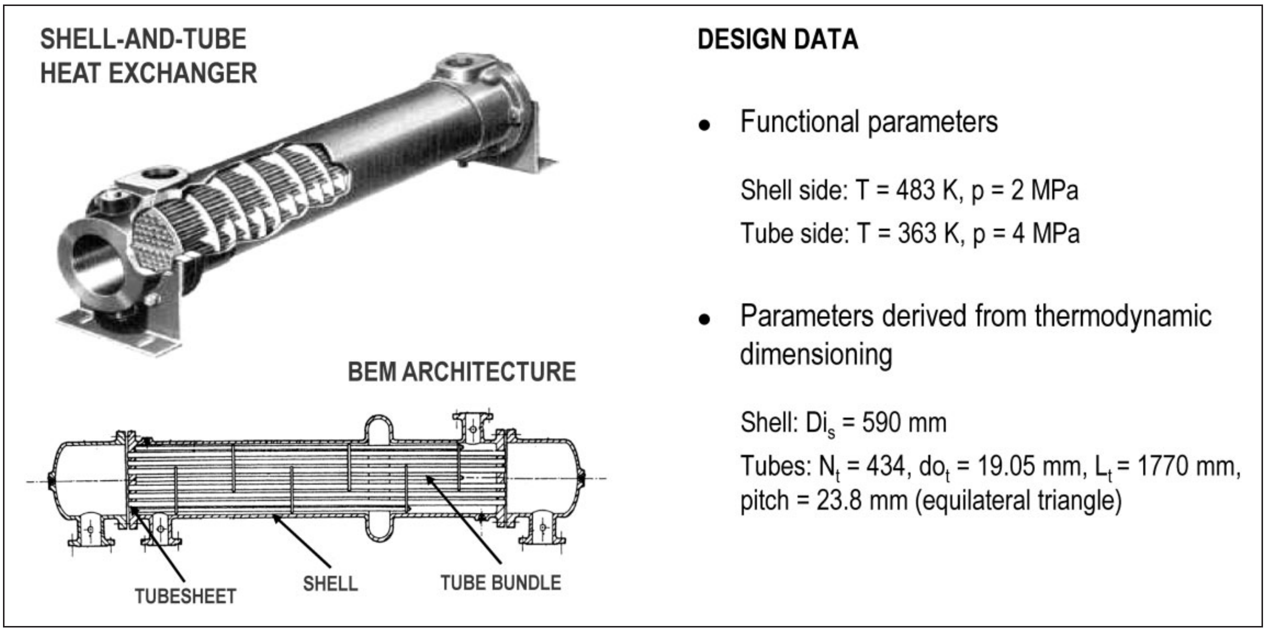

Figure 3. Application: The system and its design data.

The constraints on the variable geometric parameters $\{CoG\}$ define the limit values for the design variables to be sized, which are the thickness of the three components t_s, t_t, t_{ts}. Particularly, shell thickness t_s and tubesheet thickness t_{ts} are continuous variables, subjected to minimum value limits from TEMA standard. Tube thickness t_t is instead a discrete variable, and for the value of outer diameter fixed by the thermodynamic dimensioning, it can assume codified values between the minimum and maximum values specified in Table 2.

The constraints on the material properties $\{CoM\}$ define the primary constraints on the properties of material to be choice for each component, which are the basis for the screening of materials. In the application, the primary constraints on material properties, shared by all the components (minimum values for maximum service temperature and fracture toughness, from Tables 1 to 3) have been used for a pre-screening executed by mean of Cambridge Engineering Selector software, to obtain a pre-selection of materials (dashed box in Figure 1) to be included in the database. With this purpose, constraints on resistance to corrosion, and other sources of deterioration, have been added, as well as a maximum limit to the cost per unit mass of the material, to avoid the choice of materials not economically sustainable for the specific use.

For the whole system, the set of constraints between components $\{CbC\}$ have been defined (Table 4). In this regard, some peculiarities are noteworthy. Some constraints between components are constraints on geometric parameters, and constraints on linear and radial expansion, that are functions of material property (coefficient of linear expansion α), requirement (thermal load ΔT), and geometric parameters (length or radius), according to the generalized equation (6) for constraints between components. As can also be verified from the equations in Table 3, performance functions PF_{31}, PF_{32}, and constraints on requirements equations CoR_{31}, CoR_{32} of component C_3 (tubesheet) depend indirectly (PF_{31}, PF_{32}) or directly (CoR_{31}, CoR_{32}) on various geometric parameters of other components of the analyzed system (shell diameter Di_s and thickness t_s, tube outer diameter do_t); equation CoR_{31} depends directly also on geometric parameters of another component external to the analyzed system (head channel inner diameter Di_c and wall thickness t_c), which can, however, be traced back to geometric parameters of the component C_1 (as specified in Table 4); with particular regard to the cases of direct dependence of these equations on the properties of other components, this dependence highlights the meaning to introduce the properties of other components $O_T C_O P_R$, in the generalized form of equations (2), (3), and (7).

The performance functions of the three components, PF_{11} and PF_{12} (Table 1), PF_{21} and PF_{22} (Table 2), PF_{31} and PF_{32} (Table 3), express the primary objectives in design that consist in limiting the weight and cost. In these cases, equations of type (1) are in the form independent of requirements to be constrained RoC_{constr}. Performance function PF_{23} (Table 2), which expresses a key functionality of the component C_2 (the efficiency in heat conduction of the tubes, quantified by the heat exchange per volume unit), represents instead a typical case in which performance function depends also on requirements to be constrained RoC_{constr} (ΔT in this case). The values of PF_{21}, PF_{22}, and PF_{23} have been calculated for the

Table 1. Complete characterization of shell (C_1).

Requirements on component $\{RoC\}_1$			
$\{RoC_{opt}\}_1$		Mass m, Cost C	
$\{RoC_{constr}\}_1$		Pressure load Δp, Thermal load ΔT, Maximum bending δ_{max}	
Performance functions $\{PF\}_1$			
PF_{11}	Shell mass	$m = \rho\pi Di_s L_s t_s$	Equation (1)
PF_{12}	Shell cost	$C = c_m \rho\pi Di_s L_s t_s$	Equation (1)
Constraints on requirements $\{CoR\}_1$			
CoR_{11}	Tang stress from pressure load Δp	$\Delta p \leqslant \frac{2\sigma_y t_s}{Di_s}$	Equation (2)
		$CR_{11} = \frac{2\sigma_y t_s}{Di_s \Delta p} \geqslant 1$	Equation (3)
CoR_{12}	Tang stress from thermal load ΔT	$\Delta T \leqslant \frac{2(1-\nu)\sigma_y}{\alpha E}$	Equation (2)
		$CR_{12} = \frac{2(1-\nu)\sigma_y}{\Delta T \alpha E} \geqslant 1$	Equation (3)
CoR_{13}	Bending stiffness	$\frac{F_1}{\delta_{max}} \leqslant \frac{3\pi E\left[Di_s^4 - (Di_s - t_s)^4\right]}{4L_{a1}^3}$	Equation (2)
		$CR_{13} = \frac{3\pi\delta_{max} E\left[Di_s^4 - (Di_s - t_s)^4\right]}{4L_{a1}^3 F_1} \geqslant 1$	Equation (3)
Efficiency functions $\{EF\}_1$			
EF_{11}	Tang stress from pressure load Δp	$EF_{11} = 1/CR_{11}$	Equation (7)
Constraints on geometric parameters $\{CoG\}_1$			
	Shell thickness (TEMA std)	$t_s \geqslant 7.9$ mm	Equation (4)
	Inner diameter	$Di_s = 590$ mm	Equation (4)
	Length of the shell span between the support saddles	$L_{a1} = 1400$ mm	Equation (4)
Constraints on material properties $\{CoM\}_1$			
	Max service temperature	$Tmax \geqslant 363^\circ K$	Equation (5)
	Fracture toughness	$K_c \geqslant 15\,MPa.m^{1/2}$	Equation (5)

Δp: pressure inside the shell; ΔT: maximum temperature difference between inside and outside of the shell; δ_{max}: maximum bending allowable at the center of the shell span between the support saddles; t_s: shell thickness; Di_s: inner diameter of the shell; L_s: shell length; L_{a1}: length of the shell span between the support saddles; ρ: density; c_m: cost per unit weight; σ_y: yield strength; ν: Poisson's coefficient; α: coefficient of thermal expansion; E: Young's modulus; $Tmax$: maximum service temperature; K_c: fracture toughness; F_1: sum of the weight of the shell section between the support saddles and the weight of the fluid.

whole tubes bundle (taking into account the total number of tubes N_t).

Specificities in the implementation of the algorithm

Data restructuring introduced in section "Search for the optimal solution" consists of the compilation of the component properties vectors $CP_i = \{cp_{ik}\}_{k=1,\ldots,np}$, with n_p the dimension of the overall set of component properties introduced in the formulation of the design problem previously formalized (section "Materials distribution and components sizing problem formalization"). For each ith component C_i of the system, the CP_i vector has been compiled:

$$CP_1 = \left\{\Delta p, \Delta T, \delta_{max}, Di_s, L_{a1}, t_{smin}, Tmax_{min}, Kc_{min}, L_t\right\}$$
$$CP_2 = \{\Delta p, \Delta T, \delta_{max}, do_t, L_t, L_{a2}, t_{tmin}, t_{tmax}, \lambda_{min}, Tmax_{min}, Kc_{min}\}$$
$$CP_3 = \left\{\Delta p, \phi, pt, t_{tsmin}, Tmax_{min}, Kc_{min}, Di_s, do_t, (Di_c, t_c)\right\}$$

Table 2. Complete characterization of tubes (C_2).

Requirements on component $\{RoC\}_2$			
$\{RoC_{opt}\}_2$		Mass m, Cost C, Heat exchange per volume unit $q_{T/V}$	
$\{RoC_{constr}\}_2$		Pressure load Δp, Thermal load ΔT, Maximum bending δ_{max}	
Performance functions $\{PF\}_2$			
PF_{21}	Tubes bundle mass	$m = \rho\pi do_t t_t L_t N_t$	Equation (1)
PF_{22}	Tubes bundle cost	$C = c_m \rho\pi do_t t_t L_t N_t$	Equation (1)
PF_{23}	Heat exchange per volume unit	$\frac{q_T}{V} = \frac{\lambda}{t_t^2} \cdot \Delta T$	Equation (1)
Constraints on requirements $\{CoR\}_2$			
CoR_{21}	Tang stress from pressure load Δp	$\Delta p \leqslant \frac{2\sigma_y t_t}{do_t}$	Equation (2)
		$CR_{21} = \frac{2\sigma_y t_t}{do_t \Delta p} \geqslant 1$	Equation (3)
CoR_{22}	Tang stress from thermal load ΔT	$\Delta T \leqslant \frac{2(1-\nu)\sigma_y}{\alpha E}$	Equation (2)
		$CR_{22} = \frac{2(1-\nu)\sigma_y}{\Delta T \alpha E} \geqslant 1$	Equation (3)
CoR_{23}	Bending stiffness	$\frac{F_2}{\delta_{\max}} \leqslant \frac{3\pi E\left[do_t^4 - (do_t - t_t)^4\right]}{4L_{a2}^3}$	Equation (2)
		$CR_{23} = \frac{3\pi\delta_{\max} E\left[do_t^4 - (do_t - t_t)^4\right]}{4L_{a2}^3 F_2} \geqslant 1$	Equation (3)
Efficiency functions $\{EF\}_2$			
EF_{21}	Tang stress from pressure load Δp	$EF_{21} = 1/CR_{21}$	Equation (7)
Constraints on geometric parameters $\{CoG\}_2$			
	Tube thickness (TEMA std)	$t_t \in [0.889, 3.404]$ mm	Equation (4)
	Outer diameter	$do_t = 19.05$ mm	Equation (4)
	Tube length	$L_t = 1770$ mm	Equation (4)
	Length of the tube span between two subsequent diaphragms	$L_{a2} = 350$ mm	Equation (4)
Constraints on material properties $\{CoM\}_2$			
	Thermal conductivity	$\lambda \geqslant 50$ W/mK	Equation (5)
	Max service temperature	$Tmax \geqslant 483°$K	Equation (5)
	Fracture toughness	$K_c \geqslant 15$ MPa.m$^{1/2}$	Equation (5)

Δp: maximum pressure difference between inside and outside of the tubes; ΔT: maximum temperature difference between inside and outside of the tubes; δ_{max}: maximum tube bending allowable between subsequent diaphragms; t_t: tube thickness; do_i: outer diameter of the tube; L_t: tube length; L_{a2}: length of the tube span between two subsequent diaphragms; N_t: number of tubes in the bundle; ρ: density; λ: coefficient of thermal conductivity; c_m: cost per unit weight; σ_y: yield strength; ν: Poisson's coefficient; α: coefficient of thermal expansion; E: Young's modulus; $Tmax$: maximum service temperature; K_c: fracture toughness; F_2: sum of the weight of the tube section between two subsequent diaphragms and the weight of the contained fluid.

The specification of the terms that appear in the vectors can be found in the nomenclature at the end of Tables 1 to 4. How it is possible to observe, the properties specified by CP_i vectors consist in generalized stresses quantifying the constraints on some requirements; fixed values and/or limit values to be imposed on geometric parameters and on material properties; properties of the other components that

Table 3. Complete characterization of tubesheet (C_3).

Requirements on component $\{RoC\}_3$			
$\{RoC_{opt}\}_3$		Mass m, Cost C	
$\{RoC_{constr}\}_3$		Pressure load Δp	
Performance functions $\{PF\}_3$			
PF_{31}	Tubesheet mass	$m = \rho\pi D_{ts}^2 t_{ts}/4$	Equation (1)
PF_{32}	Tubesheet cost	$C = c_m \rho\pi D_{ts}^2 t_{ts}/4$	Equation (1)
Constraints on requirements $\{CoR\}_3$			
CoR_{31}	Stress from bending load	$\Delta p \leqslant 3\eta\sigma_y\left(\frac{t_{ts}}{fDi_s}\right)^2$	Equation (2)
		$CR_{31} = \frac{3\eta\sigma_y}{\Delta p}\left(\frac{t_{ts}}{fDi_s}\right)^2 \geqslant 1$	Equation (3)
CoR_{32}	Shear stress	$\Delta p \leqslant \frac{\sigma_y t_{ts}(1 - do_t/pt)}{0.31 D_L}$	Equation (2)
		$CR_{32} = \frac{\sigma_y t_{ts}(1 - do_t/pt)}{0.31 D_L \Delta p} \geqslant 1$	Equation (3)
Efficiency functions $\{EF\}_3$			
EF_{31}	Stress from bending load	$EF_{31} = 1/CR_{31}$	Equation (7)
Constraints on geometric parameters $\{CoG\}_3$			
	Tubesheet thickness (TEMA std)	$t_{ts} \geqslant 19.1$ mm	Equation (4)
	Holes diameter	$\phi = 19.05$ mm	Equation (4)
	Holes pitch	$pt = 23.8$ mm	Equation (4)
Constraints on material properties $\{CoM\}_3$			
	Max service temperature	$Tmax \geqslant 483$ K	Equation (5)
	Fracture toughness	$K_c \geqslant 15$ MPa.m$^{1/2}$	Equation (5)

Δp: maximum pressure difference between inside of the tube and of the shell; t_{ts}: tubesheet thickness; D_{ts}: tubesheet diameter; pt: holes pitch; ϕ: hole diameter; Di_s: inner diameter of the shell; do_t: outer diameter of the tubes; $f = \frac{17-100(t_c/Di_c)}{15}$; $\eta = 1 - \frac{0.907}{(pt/do_t)^2}$; t_c: thickness of head channel wall; Di_c: inner diameter of the head channel; $D_L = \frac{4A}{C}$; $A = \frac{\pi}{4}(0.8D_{ts})^2$; $C = 0.8\pi D_{ts}$; ρ: density; c_m: cost per unit weight; σ_y: yield strength; $Tmax$: maximum service temperature; K_c: fracture toughness.

constraint the component. Particularly, $t_{s\ min}$ is the minimum value of the shell thickness, $t_{t\ min}$ and $t_{t\ max}$ are respectively the minimum and the maximum value of the tube thickness, $t_{ts\ min}$ is the minimum value of the tubesheet thickness, $Tmax_{min}$ is the minimum value requested to the maximum service temperature, Kc_{min} is the minimum value requested to the fracture toughness, λ_{min} is the minimum value requested to the coefficient of thermal conductivity (tubes only).

Material properties database has been compiled for a set of pre-selected materials, as explained in the previous section. The data of Cambridge Engineering Selector software have been used. According to section "Search for the optimal solution", each material record is constituted by a characterization vector that collect the material identification code M_{IC} (integer number), and the values of its properties involved in the formulation of the problem, that in this applications are all the material properties that appear in the equations of components characterization (Tables 1 to 3): density ρ, cost per unit weight c_m, yield strength σ_y, Young's modulus E, Poisson's coefficient ν, coefficient of thermal conductivity λ, coefficient of thermal expansion α, maximum service temperature $Tmax$, and fracture toughness Kc. The database compiled for the reported case study includes about 250 materials.

Defining the component properties vectors CP_i, all the equations that formulate the design problem remain to be functions of the variables of the problem: the materials of system's components $\{M\}$ to be chosen, represented by their properties, and the values of the variable geometric parameters of system's components $\{G_V\}$ to be sized. These will be the variables to be optimized by the search algorithm. Therefore, the solution type consists of pairs of

Table 4. Characterization of the system (constraints between components).

Constraints between components {CbC}			
$CbC_{1\text{-}2\text{-}3}$	Constraint on shell length, tube length, and tubesheet thickness	$L_t = L_s + 2t_{ts}$	Equation (6)
$CbC_{1\text{-}3}$	Constraint on shell diameter, shell thickness, and tubesheet diameter	$D_{ts} = Di_s + 2t_s$	Equation (6)
	PF_{31}, PF_{32}, CoR_{32}, are functions of $D_{ts} \rightarrow$ depend on shell diameter Di_s and shell thickness t_s		
	CoR_{31} is a function of shell diameter Di_s		
$CbC_{1\text{-}2}$	Constraint on linear thermal expansion between shell and tubes	$\Delta L_t < k_{s-t} \cdot \Delta L_s$ ($k_{s\text{-}t} > 1$)	Equation (6)
$CbC_{2\text{-}3}$	Constraint on radial thermal expansion between tubes and holes of tubesheet	$\Delta R_t > \Delta R_{ts\_h}$	Equation (6)
	CoR_{31} and CoR_{32} are functions of tube outer diameter do_t		
$CbC_{3\text{-}OC}$	CoR_{31} is a function of head channel inner diameter Di_c and wall thickness t_c	$Di_c \cong Di_s$ $t_c \cong t_s$	

L_t: tube length; L_s: shell length; t_{ts}: tubesheet thickness; D_{ts}: tubesheet diameter; Di_s: shell inner diameter; t_s: shell thickness; do_t: tube outer diameter; Di_c: head channel inner diameter; t_c: head channel wall thickness; ΔL_t: tube linear thermal expansion; ΔL_s: shell linear thermal expansion; ΔR_t: tube radial thermal expansion; ΔR_{ts_h}: tubesheet holes radial thermal expansion.

variables, one pair for each one of the three components of the system. The first variable mt_i of each pair is the code M_{IC} that identify the material of the ith component in the material properties database, and associate the corresponding properties. The second variable of the pair is the value of the geometric parameters to be sized: for the three components of the application, the thickness t_s, t_t, t_{ts}, respectively. According the notation introduced in section "Formalizations and functionalities of the search algorithm" and Figure 2, the solution type is formulated as

$$(mt_1, g_1)(mt_2, g_2)(mt_3, g_3) \quad \text{where } g_1 = t_s,$$
$$g_2 = t_t, \quad g_3 = t_{ts}$$

Each combination of the three pairs of variables represents a potential solution of the material choice and component sizing problem. Shell thickness t_s and tubesheet thickness t_{ts} are continuous variables, quantified by real numbers. As required by TEMA construction standard, instead, tube thickness t_t is a discrete variable that should assume codified values. For this reason, in the implementation of solution type, this variable can assume integer values that correspond to the codified values of tube thickness.

Finally, the fitness function will be expressed by objective function (8) defined in section "Complete formalization of materials choice and components sizing problem", to be calculated for the values of the variables constituting each potential solutions, by means of equations (1) and (7), using the data collected in component properties vectors CP_i, and in codified material properties database. In this application the following functions, detailed in Tables 1 to 3, have been selected as the terms of the objective function (8): PF_{11}, PF_{12}, PF_{21}, PF_{22}, PF_{31}, PF_{32}, PF_{23}, EF_{11}, EF_{21}, EF_{31} (the weight coefficients α_i will be referred to these functions, ordered according to this specific sequence).

Table 5. Definition of objective function: sets of weight coefficients for the three investigations.

	PF_{11}	PF_{12}	PF_{21}	PF_{22}	PF_{31}	PF_{32}	PF_{23}	EF_{11}	EF_{21}	EF_{31}
I	0.11	0.22	0.11	0.22	0.11	0.22	0	0	0	0
II	0.12	0.12	0.12	0.12	0.12	0.12	0.28	0	0	0
III	0.05	0.05	0.05	0.05	0.05	0.05	0.10	0.20	0.20	0.20

Results

The formulation of the objective function as a weighted sum of normalized terms has been exploited to perform three different types of investigations, varying the weight coefficients. The three sets of coefficients used are shown in Table 5. The first case is that of a conventional problem (Investigation I), based on the optimization of the only functions that express the masses and costs of the components (PF_{11}, PF_{12}, PF_{21}, PF_{22}, PF_{31}, PF_{32}), giving greater weight to the minimization of terms that quantify the costs. In the second case (Investigation II), the weight coefficients for the minimization of masses and costs are equated, and the greatest weight is given to the most significant functional performance for a heat exchanger, that is the maximization of the heat exchange efficiency of the tubes, expressed by the term PF_{23}. Finally, the third case (Investigation III) maintains the maximization of function PF_{23}, and introduces the efficiency functions EF_{11}, EF_{21}, EF_{31}, with the greater weights, in the search for the optimal solution.

As highlighted before (section " Formalizations and functionalities of the search algorithm"), the characteristic of genetic algorithms is that of identifying solutions of local optimum. This implies the possibility that the same algorithm, at the same search conditions, every time it runs, can identify different local optimal solutions. For this reason, for each of the three investigations defined by the different sets of weight coefficients, 10 executions of the algorithm were performed. When different solutions arise for the different executions, the most obvious criterion to consider the best solution to be the one that corresponds to the lowest convergence value of the objective function, must be taken with caution. A solution corresponding to a higher convergence value of the objective function could however be a more "balanced" solution, i.e. able to minimize the objective function avoiding conditions of excessive imbalance between the different properties expressed by the single terms constituting the objective function. This is all the more possible, the more numerous and diversified the terms of the objective function, as this case, where the terms can reach up to 10.

The results corresponding to the different runs of the algorithm must therefore be analyzed taking into account these peculiarities of the solutions obtained by means of the genetic type algorithms, and of the used objective function. For each of the three investigation performed, a simple analysis procedure was followed that is described here with regard to the case whose results show greater variance, i.e. the Investigation III, that for which the terms of the objective function are more numerous and diversified (the full set of 10 terms selected before).

For each run of the algorithm, the convergence value of the objective function has been acquired. In Figure 4(a) these values have been reported for all the 10 runs. Figure 4(b) shows the convergence graph of the algorithm executed by MATLAB, for the first run, to which the minimum convergence value assumed by the objective function corresponds.

As can be seen from the graph in Figure 4(a), the convergence values for the 10 runs are distributed in a substantially compact manner. A simple clustering expedient can be, however, applied to define a cluster of values to be considered of particular interest (search cluster). Indicating with v_i the value corresponding to the ith run, the search cluster can be constituted by the larger set of values v_i, sorted in ascending order, starting from the lowest value v_{min} (v_1 in Figure 4(a)), such that their average value falls within a maximum limit defined by $k \cdot v_{min}$ ($k > 1$). The lower the value of k, the more compacted the cluster toward the minimum value v_{min}. In Figure 4(a), the straight line represents the average value of the search cluster defined for $k = 1.1$, and the circled values represent the elements of the cluster identified.

Each element of the cluster represents a possible optimal solution, defined by a specific combination of materials and variable geometric parameters for the three components of the system under examination. These solutions can be treated as a set of top-ranked solutions, according to the basic approach to qualitative evaluations, by means of nonstructured supporting information on materials, as suggested before (section "Formalizations and functionalities of the search algorithm"). Alternatively, to define an optimal solution among those belonging to the search cluster, a wide variety of techniques for multi-criteria decision making can be used, such as those widely applied to the basic material selection problem.[19] In this case, the simple Cartesian distance of each solution with respect to the theoretical best solution, that is the ideal solution collecting all the best values for each term of the objective function, has been used for the purpose.

In Table 6, the values assumed by the 10 terms of the objective function are reported for each solution of the search cluster (corresponding to the results for the runs 1, 3, 4, 5, 7). In the second-last column, the Cartesian distances CD calculated on the normalized values of these terms are reported. For completeness,

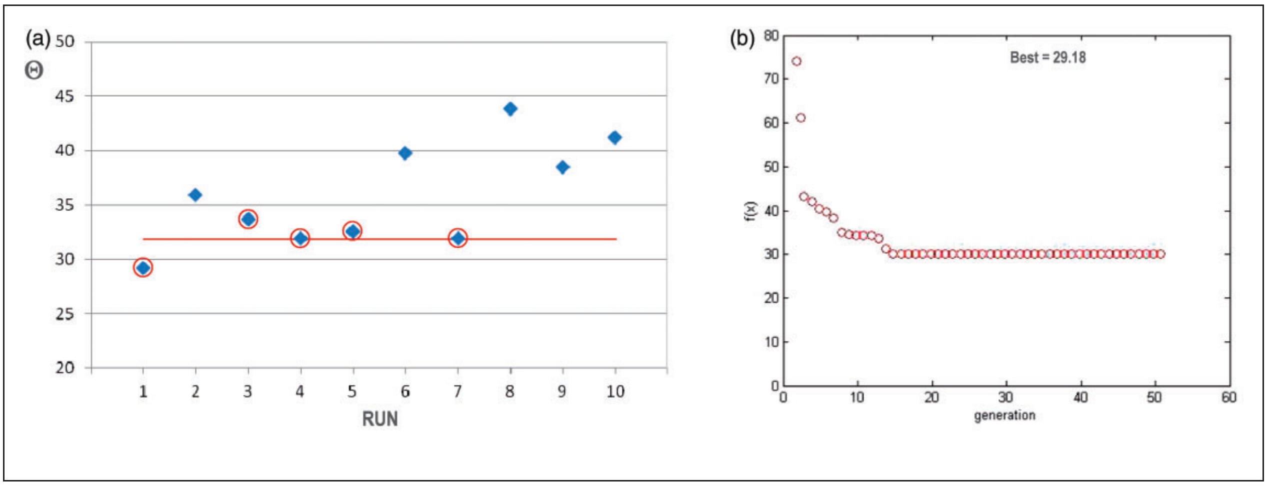

Figure 4. Results of Investigation III: (a) analysis and clustering of best solutions for each algorithm run; (b) convergence graph for first run (minimum value of objective function).

the values of similarity to the best condition SBC according to the basic TOPSIS method (Technique for Order Preference by Similarity to the Ideal Solution), frequently used in materials selection field, are reported in the last column, with identical ranking results with regard to the CD analysis (contrary to CD, the best value for SBC is the highest).

The solution obtained by run 4 is clearly the closest solution to the theoretical best solution TBS (last row), that collects the minimum values for the terms of the objective function to be minimized (PF_{11}, PF_{12}, PF_{21}, PF_{22}, PF_{31}, PF_{32}), and the maximum values for the terms of the objective function to be maximized (PF_{23}, EF_{11}, EF_{21}, EF_{31}). This is the best solution for the Investigation III, and is detailed in Table 7, together with the other best solutions obtained by applying the same procedure to the other two investigations. Each solution defines material choice and thickness sizing for each of the three components of the system analyzed.

The best solution obtained for Investigation I represents a good compromise between the traditional needs of containment of weights and costs of the components. The term relater to heat exchange efficiency (PF_{23}) obtained an acceptable value, despite being excluded from weight coefficients assignment. Efficiency functions also have not been subjected to any control during the executions of the algorithm. Consequently, their low values express inefficiency in material choice and/or component sizing.

The results of Investigation II are incisively influenced by the predominant weight fixed for the efficiency of the heat exchange. With respect to the previous investigation, the costs of the components increase. The rise in the cost of the tubes is particularly significant, but to the full advantage of the term that quantifies the efficiency of heat exchange. No significant variation can be found for the values obtained for efficiency functions, also in this case excluded from the assignment of weight coefficients.

Table 6. Analysis of search cluster (Investigation III): terms of objective function, theoretical best solution, Cartesian distances, and similarities to best condition (TOPSIS).

	PF_{11}	PF_{12}	PF_{21}	PF_{22}	PF_{31}	PF_{32}	PF_{23}	EF_{11}	EF_{21}	EF_{31}	CD	SBC
	(kg)	(€)	(kg)	(€)	(kg)	(€)	(kW/m^3)					
III	0.05	0.05	0.05	0.05	0.05	0.05	0.10	0.20	0.20	0.20		
1	351	522	418	1197	92	158	80465	0.22	0.14	0.47	0.37	0.45
3	260	418	399	1290	104	164	88066	0.30	0.15	0.39	0.28	0.46
4	**250**	**325**	**424**	**1186**	**80**	**136**	**77757**	**0.31**	**0.15**	**0.59**	**0.07**	**0.91**
5	250	311	396	1364	126	185	89159	0.29	0.13	0.31	0.39	0.31
7	249	309	430	1187	95	144	75340	0.31	0.15	0.43	0.19	0.56
TBS	249	309	396	1186	80	136	89159	0.31	0.15	0.59		

Table 7. Best solutions for the three investigations.

C_1 (Shell)			C_2 (Tubes)				C_3 (Tubesheet)		
mt_s		t_s (mm)	mt_t			t_t (mm)	mt_{ts}		t_{ts} (mm)
Investigation I									
Carbon steel AISI 1025		12.4	Carbon steel AISI 1015			1.473	Carbon steel AISI 1080		37.4
PF_{11} (kg)	PF_{12} (€)	EF_{11}	PF_{21} (kg)	PF_{22} (€)	PF_{23} (kW/m^3)	EF_{21}	PF_{31} (kg)	PF_{32} (€)	EF_{31}
326	490	0.15	515	772	47,876	0.10	88	105	0.43
Investigation II									
Stainless steel ASTM A747		9.2	Copper alloy CuAl7			1.473	Stainless steel 15-5PH		38.2
PF_{11} (kg)	PF_{12} (€)	EF_{11}	PF_{21} (kg)	PF_{22} (€)	PF_{23} (kW/m^3)	EF_{21}	PF_{31} (kg)	PF_{32} (€)	EF_{31}
244	610	0.08	522	1460	79,289	0.12	87	260	0.37
Investigation III									
Low alloy steel AISI 5140		9.4	Copper alloy CuMn13Al8			1.245	Low alloy steel AISI 4135		35.2
PF_{11} (kg)	PF_{12} (€)	EF_{11}	PF_{21} (kg)	PF_{22} (€)	PF_{23} (kW/m^3)	EF_{21}	PF_{31} (kg)	PF_{32} (€)	EF_{31}
250	325	0.31	424	1186	77,757	0.15	80	136	0.59

Finally, Investigation III provides a very interesting solution. It expresses a good trade-off between the needs to contain weights and costs, and the efficiency of heat exchange. It identifies materials choice and component sizing that ensure the best design efficiency, expressed by the higher values assumed by all the three efficiency functions (with particular regard to EF_{11} and EF_{31}), compared to the previous investigations. This last result confirms the influence that the efficiency criterion could exert in guiding the search for the optimal material-thickness coupling. Furthermore, the greater weight attributed to the efficiency functions push the algorithm to search for solutions that optimize the exploitation of the proprieties of the materials used, forcing it to identify combinations of materials and thicknesses that also entail a general containment of weights and costs.

To conclude, it is considered of interest to compare the results obtained through the proposed approach and tools (summarized in Table 7, and identified with the order number of the Investigations I, II, III), with conventional solutions that can be considered as reference (Table 8): a basic design (BD), which proposes materials conventionally used for the specific application (AISI 304 for the shell, AISI 321 for the tubes, AISI 5160 for the tubesheets), and the sizing of the geometric variables t_s, t_t, t_{ts}, obtained by traditional calculation procedures; the solutions obtained by optimizing the geometric variables only, for the three previously set investigations (according to the same weight coefficients in Table 5), keeping the basic design materials fixed (solutions BM-I, BM-II, BM-III).

In the latter case, that excludes the choice of materials, it is possible to detect some significant evidences: the optimization of the geometric variables only, has limited scope, and its results are flattened by the constraints imposed by the construction standards, specified in Tables 1 to 3 ($t_s \geqslant 7.9\,\text{mm}$; $t_t \in [0.889, 1.245, 1.473,\ldots]$ mm; $t_{ts} \geqslant 19.1\,\text{mm}$); the impossibility of changing the materials in fact does not allow to optimize the performance features, with particular reference to the cost functions (PF_{12}, PF_{22}), and even more to the efficiency of heat exchange (PF_{23}), and also limits the possibility to obtain efficient solutions, as highlighted by the analysis of the values assumed by EF_{11} and EF_{21}; finally, it results that the improvement of the design compared to the basic solution (BD) is not very significant.

In the basic design, only the choice of the material for the third component turned out to be efficient, as shown by the values of PF_{31} and PF_{32} corresponding to the Investigation BM-I, BM-II, BM-III, and the same basic design BD, and as confirmed by the corresponding values of EF_{31} also. This is a clear example of how a strictly conventional approach like the one represented by the BD solution, can lead to efficient results but limited to a single component. Furthermore, not even a systemic approach to geometric sizing, bound to pre-established conventional materials (solutions BM-I, BM-II, BM-III), can overcome this intrinsic limitation.

These observations are supported by the comparison of the values assumed by the objective function (8), for previous defined solution (materials choice and sizing optimization solutions I, II, III; fixed basic materials and sizing optimization solutions BM-I, BM-II, BM-III). With this purpose, the comparison has been differentiated by the three types of investigation (weight coefficients of Table 5). In all three cases the results were also compared to the basic design solution (BD). Therefore, the calculation of the objective function was performed separately for each investigation: e.g. for Investigation I, the set of solutions compared, with respect to which the terms of function (8) were normalized, has included I, BM-I, BD. The comparison set in this way (Table 9), has highlighted that the improvements obtained only from sizing optimizations, with prefixed materials (solutions BM-I, BM-II, BM-III), compared to the basic design that use the same materials (BD), are limited (reduction of the objective function between 13% and 22%). Moreover, they become almost negligible if compared to the drastic improvements obtained by the combined optimization of the choice of materials and sizing (solutions I, II, III): objective function reduction of about 50% with respect to the basic design, which goes up over 80% for Investigation III.

Table 8. Comparison of previous results with materials-fixed and basic solutions: materials choice and sizing optimization (I, II, III); fixed basic materials and sizing optimization (BM-I, BM-II, BM-III); basic design (BD).

	t_s (mm)	t_t (mm)	t_{ts} (mm)	PF_{11} (kg)	PF_{12} (€)	PF_{21} (kg)	PF_{22} (€)	PF_{31} (kg)	PF_{32} (€)	PF_{23} (kW/m^3)	EF_{11}	EF_{21}	EF_{31}
I	12.4	1.473	37.4	326	490	515	772	88	105	47876	0.15	0.10	0.43
II	9.2	1.473	38.2	244	610	522	1460	87	260	79289	0.08	0.12	0.37
III	9.4	1.245	35.2	250	325	424	1186	80	136	77757	0.31	0.15	0.59
BM-I	8.0	1.245	35.9	218	765	452	1718	81	65	21088	0.15	0.06	0.67
BM-II	8.4	1.245	35.2	229	802	452	1718	79	63	21088	0.14	0.06	0.69
BM-III	8.1	1.245	34.7	221	773	452	1718	78	62	21088	0.15	0.06	0.71
BD	8.5	1.245	41.3	233	817	452	1718	93	75	21088	0.14	0.06	0.50

Table 9. Results compared by the type of investigation: values of objective function (8) and improvements with respect to the basic design.

	Θ			Θ			Θ	
I	15.31	–43.3%	II	12.46	–57.3%	III	6.89	–84.2%
BM-I	21.02	–22.1%	BM-II	25.23	–13.5%	BM-III	34.77	–19.5%
BD	26.98		BD	29.17		BD	43.21	

These further results allow to propose some final concluding observations: it is confirmed that a well-structured choice of materials takes on a determined role in design optimization, and also by virtue of simultaneity, can enhance the benefits of efficient sizing, the more when the latter is strongly constrained (in this sense, the possibility of varying materials can compensate for the limitations in sizing); the impact of only sizing optimization on the performance features of the design solutions is valid, but limited regardless of the choice of materials, as the properties of the latter are crucial (in the proposed example, this is evident for the containment of the cost, and even more for the main functional performance, expressed by the efficiency of heat exchange).

In the light of the previous observations, it is confirmed that in principle a choice of materials as open as possible may be preferable, and in this sense an approach like the one proposed can enhance its heuristic value, able to investigate new unconventional solutions that can prove to be particularly efficient and widen the horizons of design experience.

Conclusions

A methodological framework and the complete and generalized modeling for a rational materials choice and sizing in multi-component design environment, have been proposed. Their potential for the optimization of simultaneous materials selection and sizing problem has been discussed, and a genetic algorithm-based approach has been presented. As a result, a structured method is provided, able to overcome the intrinsic limitations of the conventional component-level approach; avoid forcing the choice of materials within strongly limited search domains, which would affect the efficacy of final results; obtain a real concurrent optimization of the choice of materials and the sizing of geometric variables, even in compliance with the system-level constraints, and an efficiency criterion, overcoming at the same time the difficulties that the overconstrained problems entail.

The reported application, in addition to confirm the adequacy of the overall approach to the problem, has revealed further significant evidences, particularly with regard to the peculiarities of the proposed formalization and optimization approach, that converge in the formulation of the objective function as a weighted sum of normalized terms, with the well-known advantage of being able to perform different investigations, varying the weight coefficients. From investigations conducted in this way, the influence that the efficiency criterion could exert in guiding the search for the optimal material-size coupling emerges. A final comparison of the results obtained by means of the proposed approach, with reference solutions based on pre-fixed materials define by conventional design, reveals how much the impact of only sizing optimization on the performance features of the design solutions is limited, and an approach like the one proposed can enhance the heuristic potential of the search for optimal solution.

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