ARTIFICIAL INTELLIGENCE IN PROCESS DESIGN

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Summary

In this article we describe and study in detail the general activities connected with the design of thermal systems, which is the only design problem of our concern in this topic.

The problem position will be discussed first (Section 3), to analyze the various forms under which a design task can present itself to an engineer.

1. Introduction

The important point that we want to make here is that there is *one* general design protocol for all types of design problems: this point is crucial to our thesis; because it is in fact the justification for our search for artificial intelligence (AI) based “design assistants.” In Section 4, we show that the two fundamental design tasks encountered by an engineer, namely direct (simulation) and inverse (design) problems, are amenable to a single metaprocedure (optimization is not treated at length here and is the subject of *Operation Optimization of Energy Systems*, *Design and Synthesis Optimization of Energy Systems* and *Design Optimization of Power and Cogeneration Systems*). Section 5 contains a brief conceptual description of the computer-aided design tool of interest for our purposes at the present state of technology: process (or system) “synthesizers,” which are expert design assistants. Finally, three examples of applications are presented and discussed (Section 7).

2. Is There a “Universal” Design Paradigm?

The fundamental question that needs to be answered before we embark on a discussion about the possibility of implementing “expert design assistants” is the following: is it possible to construct a “universal” design paradigm to describe *every conceivable act of design*? (A paradigm is a common principle of organization that constitutes the conceptual basis for a programming language or a solution procedure. Notice that a paradigm is not necessarily algorithmic: in fact, we shall see that most AI applications to the field of thermal design are necessarily non-algorithmic.)

This question has already been answered in the affirmative in *Design and Synthesis Optimization of Energy Systems*: here, we must only recall that an essential feature of most design tasks is that *they are posed as ill-structured problems*. As discussed in detail in the quoted article, an ill-structured problem:

1. cannot be described solely in terms of numerical variables, scalar, and vector quantities;
2. possesses goals that cannot be specified in terms of a well defined objective function;
3. admits of no algorithmic solution.

Ill-structured problems are often called ill-defined, dynamic, or uncontrollable; but their most striking feature is that their solutions are *unpredictable*, in the sense that the very same design environment in which the solution is to be found has a strong influence on the existence, uniqueness, and type of solution. To solve these problems, an engineer relies on judgment, experience, heuristics, intuition, and analogy rather than on specific knowledge of solution procedures applicable per se. Actually, it is well known today that ill structured problems can be solved by some kind of structured engineering reasoning. Our interest here is that of reassessing the meaning of the term “design activity,” because if we were to compile a detailed list of the various subactivities that constitute a "design procedure," it becomes immediately apparent that all of these activities are common to almost *every* design task. There may be specific exceptions that in no way challenge the validity of the "general design procedure," of which a logical flowchart is shown in Figure 2 of *Design and Synthesis Optimization of Energy Systems*. If we accept the idea that *every* design procedure is composed of the same building blocks, we can proceed to implement a "universal design paradigm" that results in the successful solution of a specific instantiation of the universal design procedure as described in the following article. The question is not one of philosophical interest: if such a universal design procedure exists, we can attempt to mimic it with tools based on artificial intelligence structures, and create those expert design assistants that constitute the object of our search in this series of essays. This is why it is so important to properly pose our problem here: we do not advocate the use of AI tools to reproduce human thinking patterns per se, but to imitate on a simpler (fewer complexes) scale some of the mental procedures that seem to be performed in the course of a design effort. Our "expert design assistants" are thus implementations of simplified models of some specific mental patterns, and do not claim (nor aim) to be "substitute" for the human brain processes. On the other hand, we want to stress that it would be impossible to construct such models if we did not accept a somewhat reductionist representation of human thought processes. Our "model" of the human mind is non-metaphysical and somewhat materialistic: no other entities besides data and rules (the interconnections between data) are needed to justify and reproduce the thinking patterns of a designer. The remarkable success of such an approach (and the effective failure of its opposite, the "holistic" approach) justifies its adoption as a funding paradigm for our attempts. This stated, we shall deal in the following section with mere practical implementations of the general design procedure identified and discussed above.

3. Application of the Universal Design Procedure to Process Engineering Problems

3.1. Formulation and Position of a Process Engineering Design Task

An engineering task pertaining to the (partial or global) design of a thermal system is, in a logical sense, a problem generally amenable to a meta-mathematical formulation, which consists of a set of *goals*, a set of *premises*, and a set of *constraints*.

The goals are given in the form of qualitative or quantitative descriptions of the "products" of the system to be designed. They can be physical goals in a strict sense (tons of steam per hour at certain thermodynamic conditions, megawatts of installed power, liters per minute of desalinated water, etc.). Alternatively, they can be less immediately physical, but unequivocally engineering-like specifications (global efficiency of a compressor under certain well specified conditions, overall performance of a heat exchanger network, a specified value of stack emissions of certain pollutants, etc.).

The premises, also called the *design data*, consist of quantitative or qualitative information about the available inputs the engineer can use to achieve the goals (quantity and chemical composition of the available cooling water, type, chemical and physical properties of all participating media, including fuels and raw materials, information about the immediate surroundings of the proposed plant, etc.).

The constraints are usually given under the form of a list of affirmative and negative propositions about either the outputs of the process and their physical impact on its immediate surroundings, or limitations imposed on inputs, outputs, or the physical structure of the plant (pollution limitations, visual impact, environmental regulations, maximum or minimum price of either the equipment or the unit of product, social or economic limitations imposed by laws and regulations, etc.).

Ideally, an engineering task is always well-posed: that is, the inputs are completely and unequivocally specified, the outputs exactly quantified, and the constraints exactly known. This is the type of engineering design problem that is usually described in textbooks, and in fact often goes under the name of “textbook problem.” Such problems always admit at least one perfectly defined quantitative solution. They can be solved using well-defined design procedures that proceed from the premises to the goals, taking into account all constraints. They result in at least one (and usually more than one) process or system structure, consisting of a certain number of well-identified components that act on the input fluxes of matter and energy to produce the required outputs of matter and energy. There may be cases in which there is no possible solution, but they correspond to easily identified situations in which the state-of-the-art of that particular branch of technology does not allow the required input→output transformation because of limitations, usually related to the performance of one or more of the pieces of equipment necessary realizing the process. This would be the case, for instance, of a fuel-to-power transformation based on combustion with an required overall efficiency higher than 70 %, if the fuel is natural gas and the cooling medium available is air at 313 K; or, to mention a problem widely discussed at the time of writing, of electricity generation based on nuclear fusion.

Unfortunately, real world problems are seldom textbook problems: though the goals are usually well defined, data are incomplete, and often expressed in a qualitative instead of quantitative fashion, and constraints are weak, or worse yet, *vague*. (A weak constraint has the form “p not higher than C” or “q at least equal to C,” that is, “$p \leq C$” or “$q \geq C$.” A strong constraint always has the form “$s = C$.”) These cases must be handled nevertheless by the design engineer—and of course, they are, because processes are devised and plants built even under these conditions—but some of the comfortable certainties offered by textbook problems are no longer available. Therefore, there is no *a priori* certainty of the existence of even one, let alone several, quantitative solutions, because generally there is no well-defined *specific* design procedure that the engineer can follow to proceed from the premises to the goals taking into account all constraints. (This is not at odds with the thesis of this essay: while specific, that is case-dependent, particular design procedures may not be available for all types of design problems, it is always possible to formulate, tackle, and solve an engineering design task within the guidelines of the “general design procedure” outlined here.) It is true that even in these cases, there may be more than one process or system structure consisting of a certain number of well-identified components that act on the input fluxes of matter and energy to produce the required outputs of matter and energy. However, the type and performance of these structures depend on some choices the engineer must make along the way, and the results must be checked thoroughly against the specifications, to make sure that only the available inputs are indeed necessary, that all of the required outputs are indeed produced, and that all the imposed constraints have been correctly abided by.

This calls for a redefinition of the engineering design activity. Since we are searching for a general design procedure, if we accept that most design tasks are ill-posed (from a logical–mathematical point of view, it would be more correct to say that they are not completely specified, or fuzzily posed), the first step of any design procedure is that of understanding the real problem that is hidden behind the fuzzy formulation. Some authors call this incomplete formulation the *primitive problem*. However, since we will assume that all engineering problems are formulated this way, we will not need a special name for this. We reserve the name of "textbook problem" for the well-posed form of task specification, which we shall not treat at all, because its treatment will be implicitly embedded in our "general" design procedure as a special (easier) case. The premise from which the design engineer has to start is very simple: since the problem is ill-posed, a well-posed form must be devised before a solution is attempted. The strategy for this task is at best described as follows:

1. The set of inputs must be examined and "defuzzified." This means first of all that a preliminary investigation must be carried out to determine the actual inputs, their quantitative availability, their accepted chemical–physical properties, and their cost as inputs, that is, at the boundaries of the system that we are about to design. (Notice that this "cost" is not necessarily expressed in monetary units. Though this issue is a matter of some debate, it is this author's firm opinion that the proper cost to attach to both a flux of raw material or a piece of equipment ought to be its cumulative exergetic cost, expressed in kilojoules per kilogram for the streams of matter and in kilojoules per kilowatt installed for the single piece of equipment. See also *The Thermodynamic Process of Cost Formation*)
2. The goals must be similarly analyzed, and possibly redefined, so that they are clearly and completely identified: since it is often the case that a problem is over specified (but still fuzzy!), it is useful to separate *mandatory* and *accessory* goals. Mandatory goals *must* be achieved, that is, they must be included in the "criteria for success" (see *Design and Synthesis Optimization of Energy Systems*). Accessory goals can be used as "weights" to assess the *desirability* of a solution, very much as "bonus points," which may make one of the solutions more attractive than another for both designer and customer. The choice between mandatory and accessory goals can have a large impact on the structure of the resulting process, so it is necessary to exercise prudent judgment in the choice, to make use of the advice of an expert of the field, and to seek at least a partial customer participation in this activity. It is also advisable to keep track of the initial choice, and to be ready to modify it later in the design procedure, should it appear that the initial (by its nature, somewhat arbitrary) choice is likely to have a negative impact on the outcome.
3. Equally important is the correct interpretation of the constraints. The first rule (always reported as a strong suggestion in design manuals) is to take the safe route, and impose weak constraints in a strong fashion. However, if a constraint is formulated in a vague propositional sense, like for instance "taking due care that the efficiency of the compressor is the highest possible attainable under the given conditions," the design engineer must *interpret* this rule, and re-formulate it in a form that is immediately useful for design purposes. For example, "given that the stream to be compressed is air at certain (exactly specified) inlet

conditions, with the design mass flow rate *m*, and that the required pressure ratio will be between 4 and 12, the multistage compressor shall be determined by the performance curve described in the design procedure, with a maximum acceptable deranging of -1 % absolute." Clearly, this "constraint defuzzification" is a delicate task that can make the difference between a successful design and failure, and it should be performed under expert advice and discussed in advance with the customer.

3.2. Towards a General Process Design Paradigm

Once the problem position has been properly analyzed and, if necessary, reformulated, the design engineer has already gone a long way along the path towards the solution. Our idea of a "general design paradigm" would suggest that, having reached a complete and comprehensive understanding of the goals to be achieved and of the raw materials to be used, the design engineer performs a *creative act* of conceiving, critically revising, and developing to final design form one or more processes that can be used as *means* to proceed from the raw materials to the goals.

We face a semantic problem here: traditionally, the concept of *creativity* has been applied to acts of artistic or literary production, rather than to engineering activities. For these, we use instead the word *ingenuity*.

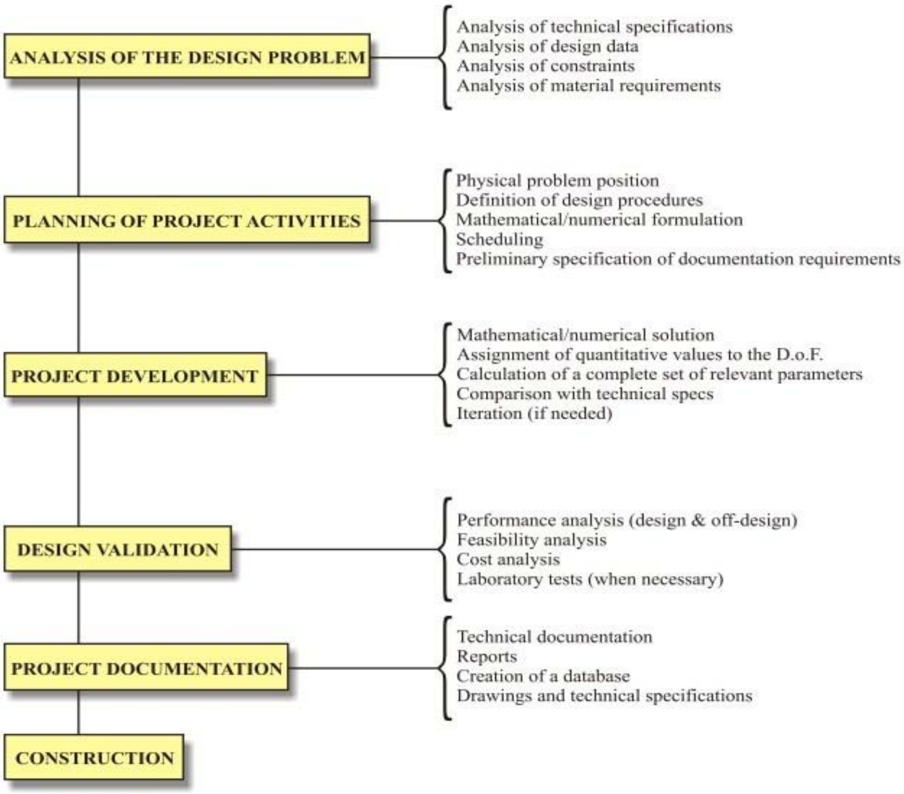

Figure 1. Process design procedure

In fact, there is no functional or mental difference between the creative act of, say, a painter and that of a process engineer: what is different in the two cases is the problem position! A work of art is originated by a *very fuzzy* problem position, in which the constraints and the goals have no need to be formulated in a precise formal way; quite on the contrary, they are more effective the more "abstract" they are (nobody would ever object to a sentence like "The artist must express himself freely."). Now we see how our "naive" idea can be implemented: the design paradigm *must* indeed begin with some creative, intuitive "concept generation." Nevertheless, the freedom that this engineering creativity enjoys in practice is not comparable to that of an act of art: in particular, there is a vast body of knowledge ("experience") that engineers avail themselves of, and that sets strict bounds both on the type and number of possible alternatives. The restraining power of this "experience" is so strong that in most instances there are very few alternative routes open for this creativity. However, this is again an inessential fact, which depends on the relatively high level of technological development at which we consider our "process design": our present technical knowledge embodies in fact all acts of past creativity, and correctly so, because nobody wants to "reinvent the wheel"!

This understanding enables us to proceed with the formulation of a general design paradigm embodying and formalizing the design procedure. Such a paradigm, which will form the basis for the subsequent application of AI techniques to process design, can be described by the following steps:

1. Consider all possible processes that can be conceivably devised to attain the goals from the premises; usually, it is convenient (though not necessary) to proceed from the simplest (fewer components) to the more complex process, because an engineer's knowledge base is by its own nature additive. (Actually, all design procedures based on simulated annealing (see *Design and Synthesis Optimization of Energy Systems*) proceed from the most complex to the simpler process configuration.) It is important that these processes be listed in an orderly fashion, with a ranking expressed by a well identified parameter, regardless of their known "implementability" from past experiences.
2. Perform a detailed conceptual analysis of some of the configurations that seem more "promising," based on past experience, external advice (including the customer's), or educated engineering intuition. It is likely that by doing so, additional configurations may be discovered, which can be obtained from the previous ones by "perturbation," that is, by adding, deleting or modifying one or more components, while keeping the general process structure unchanged. In particular, it is important that all configurations retained in the list at this point satisfy all mandatory goals. Review the list originally compiled, pruning the most complex or apparently less feasible configurations and adding some of the new ones. At this level, all choices are qualitative, or at the most semi-quantitative, because these two first steps are substantially based on the engineer's experience and creativity.
3. Screen the new list critically, with the goal of reducing the alternatives to only a few ones, so that quantitative calculations can be performed on all of them. The screening criteria ought to be based on the constraints contained in the problem formulation, and on any accessory constraint that the engineer may deem appropriate at this time (for instance, socioeconomical or technological situation of the area in which the process will be implemented into a plant, or known availability of some components on site).

4. Having reduced the alternatives to a "small" number (determined by the amount of resources that can be committed to this preliminary feasibility study), perform a preliminary calculation of the simplified process (neglecting, for instance, pressure losses in pipes and valves, secondary heat losses to surroundings, etc.). Compute efficiencies, specific fuel consumption, and any other coefficient of performance that may be of interest; also, perform a preliminary sizing of the major, non-standard equipment. Discard all configurations that result in unusually over or undersized components, that have exceedingly low efficiencies or low reliability, or that have a much larger environmental impact than the others: in practice, discard all configurations that have the least (defined in some sense) probability to achieve a desirable total of accessory goals.
5. Formulate an objective function (which may include, but ought not to be limited to, economic considerations) to assess the "goodness" of the process we are designing. Perform a more refined process simulation, and compute this objective function at design and (if necessary) at off-design conditions. Select the few alternatives for which this objective function clearly attains its "optimal" values, and repeat the refined process simulation for each one of them, under realistic operational conditions (load-following transients, start-ups and shut-downs, varying external conditions). If enough data are available, perform a life cycle analysis.
6. Select a final number of two or three alternatives and review them critically in detail, together with the customer and field experts. Once the "final" configuration has been agreed on, proceed with detailed design and operational numerical simulations.

This list applies equally well to the design of an automobile or a water desalination plant. Naturally, there are substantial differences both in the technical details and in the technological state of the individual components, but these differences can be addressed internally to each step, and do not detract from the generality of the "main" procedure, which is, in effect, *a metaprocedure applicable to all process design activities*. The flowchart of Figure 1 represents the various "tasks," each expanded in its subtasks for ease of comprehension: notice that the entire process design procedure covers steps 6, 8, 9, and 11 of the universal design procedure outlined in *Design and Synthesis Optimization of Energy Systems*.

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Biographical Sketch

Enrico Sciubba is professor at the Department of Mechanical and Aeronautical Engineering of the University of Rome 1 "La Sapienza" (UDR1), Rome, Italy. He received a masters degree in mechanical and electrical engineering from UDR1 in 1972. From 1972 to 1973, he was a research assistant at the Chair of turbomachinery in the same university. From 1973 to 1975, he worked as a research engineer in the Research and Development Division of BMW, Munich, Germany, where his tasks included the design, development and testing of advanced i.c. engines. After returning to UDR1 as a senior research assistant from 1975 to 1978, he enrolled in the Graduate School of Mechanical Engineering majoring in thermal sciences at the Rutgers University, New Brunswick, NJ, USA, where he was granted his Ph.D. in 1981. From 1981 to 1985 he was assistant professor at the Catholic University in Washington D.C., USA, teaching thermal sciences. He returned to the Department of Mechanical and Aeronautical Engineering of the University of Rome 1 "La Sapienza" (UDR1) as a faculty member in 1986. He lectures on turbomachinery and energy systems design, in both master and Ph.D. level courses. His research activities are equally divided in three main fields: Turbomachinery design and CFD applications; energy systems simulation and design; applications of AI (artificial intelligence) related techniques and procedures to the design, synthesis and optimization of complex energy systems. His publications include more than thirty journal articles (mostly on international refereed journals in the field of energy and applied thermodynamics), and over eighty refereed papers at international conferences. He has published one book on AI applications for NOVA Science, USA, and is writing a turbomachinery book for J. Wiley and Sons. Dr. Sciubba is associate editor for three major international journals in the field of energy conversion, and a reviewer for several more.