MODELING AND SIMULATION METHODS

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Summary

Traditionally, the design and operation of energy systems was based primarily on the designer's experience. The ever growing complexity of contemporary systems and the ever more stringent need to satisfy several objectives, often conflicting with each other (low cost, high efficiency, low environmental impact, and so on), make it necessary to

use automatic procedures to ease the designer's task. An overview of available computer-assisted methods is presented in order of increasing complexity. Open problems, debated issues, and further directions for research and development are also discussed.

1. Introduction: "Modeling" versus "Simulation"

Though often confused even in the specialist literature, "modeling" and "simulation" are two distinct aspects of the design problem:

- *Modeling* is the act of interpreting a set of physical phenomena and of devising a reasonably complete, closed, and comprehensive mathematical formulation for its description. Such a description usually results in a system of equations that, given a suitable set of initial data, can be solved to yield the values of the independent variables that describe the physics of the phenomena subject to modeling. It is convenient that a model be "closed," that is, that it does not require assumptions external to the theory. However, since the physics of nature is complex, this is in many instances impossible, and some "closure parameters" (semi-empirical coefficients that appear in some of the constitutive relations) are needed to close most models in a mathematical sense. Modeling is a dynamic concept: the improvement of our comprehension of the physics underlying a certain set of phenomena leads to successive refinements of the pristine model resulting in a more general, or more precise, agreement with the reality of a process. A model can also be seen as a paradigm of reality, in the sense that it expresses our interpretation of a myriad of interrelated micro and macro effects that constitute the (in principle, unknown) real process.
- *Simulation* is the act of putting our models to work. On the basis of some suitable initial data about the state of the universe, a proper mathematical formulation deriving from the model is applied to obtain the numerical values of all relevant variables for the problem in a particular case. A single model can be applied in a variety of "simulation modes," depending on the perspective under which we wish to carry out the design.

2. A Brief History of Energy Systems Design Procedures

Energy conversion systems have been in use since the late Bronze Age, and there are well-documented examples of relatively advanced devices constructed 4000 years ago. In Mesopotamia (the region presently spanned by modern Iran and Iraq), wind-to-mechanical energy conversion performed by means of primitive, but very ingenious, windmills provided the motive power needed for milling wheat. Similar windmills were known throughout the eastern Mediterranean area, and possibly even in India and China. For the same purpose, Babylonians and perhaps also ancient Indian civilizations performed hydraulic-to-mechanical energy conversion via rudimentary water wheels. Even thermal-to-mechanical energy conversion was enacted: the drawings by Hero (second century BC) show that an impulse steam turbine was in use in Egypt at least as far back as the fifth century BC. The design of such devices was certainly non-systematic, trial and error being the common design technique. The "engineers" of that time were regarded rather as magicians; they constituted a closed social class and passed their experience from generation to generation without leaving any written physical explanation of the phenomena they were exploiting. In modern terms, we can say that they did not leave records of the models they used: of course, there was not even the notion of simulation. Roman engineers, for instance, left no written record of their design practices for any of the many hydraulic plants they built. It was only after the Middle Ages (roughly, after 1300) that the first "scientific" explanations were attempted: we could say that "modeling" was born then.

From the fifteenth to the seventeenth century, windmills, watermills, and some rudimentary thermal systems (gunpowder was brought to the West from China after the year 1400) were developed, always on a trial and error basis, but often with extraordinary insight on the part of individual inventors. Design was still based on an elementary modeling activity, and no simulation was even conceived. Things changed substantially after the development of the first steam engines in the second half of the eighteenth century: the science of thermodynamics was born, and the extraordinary pace of development of the original concept in literally hundreds of applications reveals a titanic effort on the part of engineers to understand the underlying physical principles, and to concoct a "model" of their systems. Heat transfer began to be understood, and strenuous modeling activity began. Concepts such as latent and specific heat, energy transfer by conduction and convection, and fluid motion were intensely studied in the eighteenth century: of course, this required a strong modeling activity. If we examine the construction details of the machines of that age, we see that the physics of several phenomena (leakages, fluid motion, mechanical friction, and so on) were quite well understood, in that proper models were used in the design and operation of the systems.
From the mid-eighteenth to the early twentieth century, the fundamental works of Lavoisier, Carnot, Gouy, Stodola, and many others led to an evermore exact understanding of the physical laws governing the phenomena of heat and work transfer, and modeling became a scientific activity, based not only on intuition but on exact and physically sound rules involving mass and energy balances, and even consideration of irreversible losses.

In the twentieth century, emphasis was put on the organization of the large body of experimental evidence previously acquired, and models became systematic: that is, based on universal conservation equations and on the proper application of general thermo-physical property relations. Processes and systems (notably, chemical and thermal) were designed on the basis of ever more refined models of the underlying phenomena, and design procedures were devised that made use of the mathematical formulation of these models to derive (by hand calculation!) some of the independent variables. Simulation was born and immediately adapted to those rather inefficient tools: iterative calculations were reduced to a minimum, and widespread use was made of abaci and tables for relating one design variable to another. Only after the computer made its appearance in the engineering world (the event can be dated to1936, when the first "electronic" computer, the Z1, was switched on by Konrad Zuse in Saarbrucken) was it was possible to transfer the tedious load of iterative calculations from humans to machines. It became immediately apparent that computer-assisted procedures were more precise, less prone to casual error, and much faster than human calculations. The age of the slide rule came to an end, and the computer became a necessary design tool for process and design engineers.

In recent decades, the performance of every computing device has been growing at an impressive pace: number of operations per unit time (FLOPS), storage size (working "memory"), input–output devices, reliability and portability, and user friendliness have reached levels today that were almost unthinkable in the late 1980s, and progress is made literally every day. This led of course to the development of specific engineering applications. Computer tools are now available for process simulation, for the design (sizing) of components and structures, for process monitoring and control, and so on. The trend has accelerated to the point that it is difficult today to perform a flow-sheet activity (or any kind of design calculation!) without some sort of computer aid. Recent developments include the complete automation of simulation procedures and the shifting of some of the modeling activity from the human mind to the artificial assistant (see *Artificial Intelligence in the Design of Energy Systems*). Computer procedures are presently used for the solution of inverse (design) and direct (optimization) engineering problems, and the trend is clearly towards the codification of the "creative" portion of the design activity into some sort of "intelligent" code.

3. Modeling

In a logical sense, modeling (as defined in the introduction) consists of two separate activities. The first is a task pertaining to the meta-mathematical formulation of a problem (the mapping of some physical phenomena and of their relevant interconnections onto a conceptual scheme of mutually coupled processes), while the second pertains to its mathematical formulation (the problem description in computable terms). A model represents a reasonable description of the way the process or system under consideration "behaves," that is, operates under both normal and unforeseen circumstances. The three necessities of the logical construct "model" are:

- an exact knowledge of all inputs (means) and outputs (goals),
- a physical operational scheme of the component or process, and
- a functional operational scheme of the component or process.

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 usually described in textbooks, and in fact often goes under the name of "textbook problem." Its modeling invariably appears to be simple and almost univocal, as if there was only one correct way to represent the underlying physics. Unfortunately, real world problems seldom resemble textbook ones: 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. The design engineer must nevertheless handle these cases, but some of the comfortable certainties offered by textbook problems are no longer available: in particular, there is no *a priori* certainty of the validity of any "obvious" model. There may be more than one process- or system structure acting on only slightly different sets of input fluxes to produce the required outputs, and the type and performance of these structures depend in a "logically non-linear" fashion on the features of the model we adopt. In conclusion, from a logical-mathematical point of view, most design tasks are ill posed. This means that:

- the problem cannot be described solely in terms of numerical variables, scalar and vector quantities,
- it possesses goals that cannot be specified in terms of a well-defined objective function, and
- it admits to no algorithmic solution.

Ill-posed problems are often called ill-defined or ill-structured, and their most striking feature is that their solutions are unpredictable, in the sense that the environment in which the solution is to be sought has a strong influence on the solution's existence, uniqueness, and type. 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*. If we compile a detailed list of the various sub-activities that constitute the engineering portion of a design procedure, it becomes immediately apparent that all of them are common to (that is, must be performed in the course of) almost every design task. There are several ways in which these activities can be systematically classified, and the one chosen here is based on their subdivision into an initial modeling action followed by a series of calculations which constitute the simulation task.

The starting premise for the design engineer is very simple: even if the problem is ill posed, a well-posed model must be devised before a solution is attempted. The strategy for this task is at best described as follows:

- The set of inputs must be examined and de-fuzzified.
- The goals must be similarly analyzed, and possibly re-defined, so that they are clearly and completely identified: since often a problem is over-specified (but still fuzzy!), it is useful to discriminate between "mandatory" and "accessory" goals. Mandatory goals *must* be achieved, while accessory goals may be considered as "bonus points" that increase the *desirability* of a solution. The choice between mandatory and accessory goals can have a large impact on both the structure of the resulting process and its modeling, so prudent judgment is required.
- Equally important is the correct interpretation of the constraints. A first rule is that of imposing weak constraints in a strong fashion. A second rule is that of interpreting (that is, replacing with explicit expressions) all constraints formulated in a vague propositional sense: "the efficiency of the compressor must be the highest possible under the given conditions" becomes "$\eta_{\text{comp}} > 0.87$ for the given values of the inlet p and T, of the compression ratio, and for the specified flow rate and physical conditions of the process fluid."

Once the problem position has been properly reformulated, and acting on the basis of a complete and comprehensive understanding of the goals of the system, of the available inputs and of the plausible physical flows of matter and energy in the conceptual process, the design engineer performs a *creative act* of conceiving, critically revising, and developing to final form a comprehensive model of the entire process. A model is thus actually constructed via some creative, intuitive "concept generation." Of course this engineering creativity is strongly delimited by the vast body of established knowledge and verified experience available that sets strict bounds on both the type and the number of possible alternatives: this limiting action is more severe for technologically mature processes and components.

It is not possible to provide a list of modeling techniques, since obviously much is left to the insight of the single scientist or engineer: but it is possible to extract the common traits that a model ought to possess.

- A model must respect *all* known conservation laws for the quantities involved in the process. Mass and energy conservation are obvious examples, as well as dynamic quantities like angular momentum, kinetic energy, and so on.
- Whenever a certain fundamental conservative quantity is not conserved, the model must account for the relevant “dissipation”: in mass flow rates balances, leakages and the applicable leakage models must be included; in energy balances, the proper irreversibilities must be modeled, and the same applies to species conservation, and so on.
- A model ought to be based on the smallest possible set of independent variables consistent with the degree of complexity of the model itself. For example, it is advisable that mass leaks through a gap be related to the gap characteristic dimensions, to the pressure differential across it, to the quality of the surface finishing, and to the fluid viscosity, but not to non-local quantities like a reference pressure and the overall size of the component. This can be seen as a direct application of the “Ockham’s razor” principle; the thirteenth-century Oxford philosopher wrote: “*Frustra fit per plura quod potest fieri per pauciora*” (“It is useless to achieve with many [entities] what can be achieved with fewer ones”).
- A model ought to be formulated in the simplest possible mathematical way, but not in terms that are so simple as to mask important effects. For instance, since the conservation of total enthalpy in a turbo machinery passage is known to be expressed in terms of a differential equation, it is incorrect to try to reformulate it in terms of an approximate algebraic expression, which does not possess the ability to account for gradients. (“Keep things simple. But not too simple.”)
- A model should avoid as much as possible the use of “empirical closure constants.” In most cases, it is convenient to include additional equations that express the “constant” in terms of one or more physical variables for which a balance law is known to apply.
- It is convenient, whenever possible, to formulate a model in dimensionless form. By proper use of dimensional analysis, the phenomena under study can be classified into “ranges” in which the phenomenological evidence shows different patterns depending on the value of one or more dimensionless parameters (like the Reynolds, Mach, Prandtl, and Nusselt numbers) that define “attractor points” in the vicinity of which the process behaves with distinctive features that can be exploited in the model formulation. Such dimensionless numbers condense a large amount of physical information into a small set of numerical values or ranges, and are therefore a very powerful method of classifying reality.
- Finally, no model ought to be regarded as “absolute.” Following Karl Popper, we must always be conscious that a model is valid and applicable until it becomes “falsified” by an instance in which it is demonstrated that its

application leads to unreasonable results. New (more refined, but sometimes even simpler) models can be generated by examining these counterexamples.

3.1. Thermo-Physical Material Properties

The first step to make process modeling and simulation less dependent on human resources is that of developing proper models for "material properties" that provide the thermodynamic quantities of interest (enthalpy, entropy, saturation values, steam quality in the wet region, specific heats, and so on). Such models must be developed on the basis of a sound physical interpretation of the micro and macro-scale phenomena that can be *specific* for the particular fluid under consideration, or of *general validity* for a certain set of fluids, and must be obviously based as much as possible on sound and properly organized experimental evidence. Property models result in calculation routines that provide the quantities of interest in terms of a set of "fundamental quantities," usually chosen as those more easily measurable (pressure and temperature, species composition and physical state). These routines are presently available for almost all materials, and offer a high degree of accuracy and a relatively high efficiency. They can be used in either "manual" mode (that is, by plugging into them the values of the known parameters and deriving the outcome), or in "automatic" mode (that is, by using them on some kind of numerical procedure). Since the degree of accuracy depends substantially on the complexity of effects included in the model, care should be exercised to adopt the most convenient model for the use that we have in mind. Thus, a simple ideal gas law (perhaps corrected by the compressibility factor) ought to be adopted in hand calculations, while more complex relations are to be left for computer-aided applications.

3.2. Passive Components

A passive component is a unit whose purpose is *not* that of exchanging energy with the material stream(s) with which it interacts. Examples of passive components are pipes, valves, reservoirs, containers, and solid handling devices. These components are modeled by simply computing their power requirements on the basis of mass and energy conservation and including dissipative effects. Thus, a pipe conserves the mass of the fluid flowing through it, but dissipates a frictional energy proportional to the square of the volume flow rate and to the viscosity of the fluid. A model constant is necessary, like for instance the friction coefficient that can be expressed in terms of the Reynolds number of the flow and of a dimensionless roughness parameter of the pipe surface. Similar considerations apply to valves of all sorts (including rupture diaphragms and relief valves), to orifices, nozzles and ejectors, funnels, and so on. For reservoirs and containers, a mass balance prescribes that the difference between the outflowing and the incoming mass flow rates must be equal to the mass accumulation within the container. If necessary, an energy balance based on the conservation of the thermal capacity of the system allows for the calculation of the average temperature of the material within in terms of the temperature of the incoming flow. Solid handling devices that affect transport of a given mass of material require a power that is given by the displacement work times the gross mass flow rate of the material (leakage models might be employed if necessary). Stirrers and mixers require a more careful modeling, because in addition to the mass and energy balances we need to model the mixing losses and the power required to stir the material, both of which are strongly case dependent.

3.3. Active Components

An active component is a unit whose purpose is that of exchanging energy with the material stream(s) with which it interacts. Examples of active components are heat exchangers, combustors, chemical reactors, distillation towers, turbo-machines, rotary machines of all kinds, and reciprocating displacement machines. Active components are more difficult to model than passive ones, because their energy exchange mechanisms are often the result of a complex combination of elementary phenomena. In some cases (notably, chemical reactors and turbo-machines), the mass flow rate and the energy exchange are interdependent. Thus, case-by-case modeling is necessary. As a rule, mass and energy conservation laws must be supplemented by a model that relates the physics of the phenomena to a “typical” set of design parameters, different for different devices. The models of these components make extensive use of dimensionless parameters expressing the material properties (*Re*, *Ma*, *Pr*, *Nu*, and so on), and of “characteristic curves” of the component, derived either on the basis of prime principles (the fundamental exchanges between machine and fluid) or on experimental evidence. More often, these characteristic curves are a combination of the two: their basic shape is derived from first principles, while their practical “engineering” shape is obtained by modifying the former by (semi) empirical shape factors. For most modern components models are actually derived from numerical simulations of the inherent physics: this is not at odds with the claim we made above, according to which “simulation” follows “modeling.” The results of the numerical computations that “simulate” the behavior of combustors and turbo-machines are treated exactly like experimental evidence: they are used to construct a (higher-order) physical model of the component’s behavior, to extract correlations among design variables, and so on.

3.4. Control and Monitoring Systems

The latest generation of process simulators includes features to treat the so-called “process auxiliary systems,” which include refrigeration, lubrication, space conditioning, and control and monitoring systems as additional plant components. The modeling of these systems can be generated with minimal effort, because they usually consist of relatively simple subcomponents (sensors, transducers, valves and switches, pipes, displacement pumps, fans, and surface heat exchangers). Though the interconnections and interactions between these components are usually steered by electronic systems, it is advisable to rely on the producer’s data rather than trying to generate an *ad hoc* model.

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Biographical Sketch

Enrico Sciubba (born 1949) is Professor in the Department of Mechanical and Aeronautical Engineering of the University of Roma 1 "La Sapienza," in Roma, Italy. He received an M.Eng. degree in Mechanical Engineering from the University of Rome in 1972. After working for two years (1973–1975) as a Research Engineer in the Research & Development Division of BMW, Munich (Germany), he returned to the University of Roma as a Senior Researcher (1975–1978). He then enrolled in the Graduate School of Mechanical Engineering, majoring in Thermal and Fluid Sciences, at Rutgers University, Piscataway, NJ, USA, where he was granted a Ph.D. degree in 1981.

He joined the Department of Mechanical Engineering of the Catholic University of America, in Washington DC, USA, as an Assistant Professor in 1981, and worked there until 1986, when he returned to the University of Rome, first as a Lecturer, then as an Associate, and finally Full Professor. He holds the Chair of Turbomachinery, and lectures on Energy Systems as well, both at the undergraduate and graduate level. In 1999 Dr. Sciubba was elected a Fellow of the American Society of Mechanical Engineers. In 2000, he also received a Honorary Doctoral title from the University Dunarea de Jos of Galati (Romania). His research is related to CFD of Turbomachinery, to Exergy Analysis, and to Artificial Intelligence applications in the design of Energy Systems.

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