Numerical models and modeling environments: tools to effectively mobilize the scientific knowledge

R. Gicquel

INTRODUCTION

Even if, like other executives, they must increasely take into consideration non-technical dimensions of their work, that is to say, people management, economics of projects, product marketing, environmental impact of technologies ... their scientific and technical knowledge and ability to mobilize them to solve concrete problems are among the most distinctive characteristics of engineers.

The objective of this presentation[1] is to get students to think about this central aspect of the profession of engineer: the place of science in his work, and how to mobilize it effectively.

Numerical modeling is thus increasingly at the heart of the profession of the engineer, whose work environment has changed significantly in recent years and will continue to do so in the future. Increasingly, he will have automated tools to facilitate his work and especially to enable him to perform scientific calculations with greater precision than before and a significant time savings. This development, which seems irreversible, has the effect of substantially change the very work of the engineer. It is less important than before that he knows in detail how the calculations are made, **but it is essential that he knows use the results provided to him by software**, while also being able to criticize and to know their limits.

The idea is: the information and communication technology (ICTs) are revolutionizing the methods of acquisition, accumulation and transmission of knowledge. Under these conditions, the engineer less often directly manipulates equations. He uses computer models that can encapsulate and implement them effectively with powerful modeling environments.

In support of this idea, we will first briefly introduce how to develop a model for **calculating the thermodynamic properties of ideal gases** in the Java environment, allowing us to show what can make a suitable modeling environment.

Indeed, beyond the immediate resolution to a problem, modeling, if it is to be effective, must aim to be economical, safe and reusable. Based on work in this area in recent decades, it appears that this implies that the model is modular (note that the etymology of both words is the same), and the assembly of complex models is facilitated by appropriate tools: computational environments.

The problem of designing such a powerful and generic from basic well-chosen modules is very different from the design of the modules themselves. In fact, one can show that the whole uses a dual approach, globally **systemic**, and **analytical** at the level of each module.

These two approaches, often presented as contradictory, in reality prove highly complementary in this case. This requires:

• first identifying all the basic concepts necessary to solve a given class of problems. This raises the question of genericity: how, from a small number of basic primitives, to generate a large number of cases. What are the basic features that should be available... The answer to this question is primarily a systems approach
• second, primitive types being identified, how to establish the corresponding models. The approach here is essentially analytical, the connections and interrelationships between the modules being ensured by coupling well-chosen variables

[1] It is largely based on reference [9] initialy presented in 1992

A good modeling environment thus consists firstly of a set of primitive types, forming a sufficient basis for the generation of as many projects as possible, and also an interface to easily link each of these primitives to represent the objects studied, and with additional functionalities, especially for archiving.

We will develop in a second time the issue of **building numerical models**, reviewing the different types of scientific models and their mathematical translation.

We will then deal with **systemic analysis** to show what are the available theoretical bases and draw some conclusions about how to structure the modeling approach.

TYPES OF PROBLEMS

The problems most oftenfaced by the design engineer can be grouped into three broad categories: design of new devices, control of existing systems, component characterization.

The design of new devices:

When trying to design a somewhat complex device, it is usually impossible to be a priori certain of its operation, especially if the operating conditions are somewhat restrictive. Three classes of problems can be identified here:

• The compliance audit is to ensure that the system under study meets the specifications defined by the client. This phase, which has always been important, is now becoming essential for a class of problems where non-compliance of the specifications may result in the outright inability to carry out the planned mission, and not just a loss of efficiency. This is the case in a large part of the aerospace field.

• Optimization is an additional degree of complexity: not content to ensure compliance with specifications, the engineer then seeks to minimize a criterion that can be a combination of investment and operating costs.

• The control of the device is a complementary approach. The system being designed, it is to find a satisfactory way to control. An entire chapter of the control science is opening here... Note that, increasingly, we seek to define the control while the architecture of the system is developed. This is called a generalized design.

Control of existing systems:

When the system exists and the goal is to run it at best, the problem arises in different terms:

• First, it is necessary to observe it in order to understand its behavior, and if possible to identify a model that represents it well.

• Then, the system being properly observed, the control itself must be defined, which refers to the previous point.

Characterization of components:

In this case, from a series of appropriate experiments, we seek to determine the performance of a component or a subset, that it is not possible to isolate from the entire system, for various reasons, including physical. The techniques to be employed here are the inverse methods, or identification.

Among these three categories, it is certainly the design of new devices, including the desire to optimize performance, control included, which is the type of problem most frequently encountered. Indeed, the aim is to increasingly improve competitiveness, may it be expressed by an energy saving, increased comfort, reduced operating costs, reduced mass...

1 IDEAL GAS MODEL IN JAVA ENVIRONMENT

1.1 Equations used:

The equation of state of an ideal gas can be written: $pv = rT$

with $r = \frac{R}{M}$ (kJ kg^{-1} K^{-1})

R is the universal constant = 8.314 (kJ kmol^{-1} K^{-1})

M is the molar mass of gas (kg kmol^{-1})

The thermal capacity of an ideal gas is not constant, but depends only on the temperature.

In most cases, Cp is represented by a polynomial fit in T, such as:

$$Cp = A + B\,T + C\,T^2 + D\,T^3 + E\,T^4 + \frac{G}{T^2} + \frac{K}{T}$$

The equations of thermodynamic state functions are:

Internal energy: $u - u_0 = \int_{T_0}^{T} Cv(t)\,dt$

Enthalpy: $h - h_0 = \int_{T_0}^{T} Cp(t)\,dt$

Entropy: $s = s_0 + \int_{T_0}^{T} \frac{Cv(t)}{t}\,dt + r \ln \frac{v}{v_0}$ or $s = s_0 + \int_{T_0}^{T} \frac{Cp(t)}{t}\,dt - r \ln \frac{p}{p_0}$

All of these elements is a representation of ideal gases. To turn it into a model, we must make the translation of these equations in an appropriate computer language, together with all relevant data.

For example, object languages is a form of encapsulation of particular interest because they bring together in one object, called a class, all the elements related to a programming model: data, variables, and methods, part of the latter being accessible from the outside, while others are hidden to users.

1.2 Sketch of class GazIdeal

In our example, the class GazIdeal is characterized by:

- as data, the coefficients A-K for different pure substances and their molecular weight
- as methods functions for calculating the thermodynamic properties of interest
- for compound gases, the functions translating the Dalton law and providing the mixture values from those of the constituents.

Once the model is developed, it actually encapsulates the corresponding knowledge, and allows one to mobilize them very easily.

For clarity and brevity, the variables and methods for calculating compound gases have been removed, and the data are provided only for air and argon. The code is printed in italics, the explanations are in standard characters.

```
/**
* Class for pure and compound ideal gases
 *
 */
public class GazIdeal {
```

The class includes first variable declarations. Their range depends on their use: here, only V, H, S, Cv, U and PCI are accessible from outside the class

```
public double V,H, S,Cv, U,PCI;
private double A,B,C,D,E,F,G,K;
double   hf0,sf0,h0,s0,T0;
```

The role of the constructor is to make the initializations. Here it calls method setPropPur() for a pure gas, which makes the initializations.

```
/**
 *  GazIdeal constructor
 */
public GazIdeal(String nom_gaz, boolean pur)
{
        if(pur)setPropPur(nom_gaz);
        else setPropComp(nom_gaz);
}

/**
* Initialization of pure gases
 * @param nom_gaz String
 */
private void setPropPur(String nom_gaz) {
        if(nom_gaz.equals ("air")){
                M=28.9577634;
                A=11.664138786;B=16.548507822;C=-5.699923263;D=0.495033642;
                E=0.072122872;G=-0.094562097;K=1.690130579;
                hf0=0;sf0=192.727499;h0=0;s0=4.68226591855872;
                PCI=45720.110799;
        }

        else if(nom_gaz.equals ("Ar")){
                M=39.95;
                A=12.471;B=0;C=0;
                D=0;E=0;G=0;K=0;
                hf0=0;sf0=0;h0=0;s0=0;
        }
}
```

The methods for calculating the thermodynamic properties are as follows:

```
/**
* This method calculates the molar internal energy
 * @return double
 * @param T double (K)
 */
public double u_gaz_mol(double T){
 double $T=T/1000;
```

```
 double $u=0;
          $u=A*($T-0.298)+(B/2*($T*$T-(0.298*0.298)))+(C/3*($T*$T*$T-(0.298*0.298*0.298)));
          $u=$u+(D/4*($T*$T*$T*$T-(0.298*0.298*0.298*0.298)))+(E/5*($T*$T*$T*$T*$T-
(0.298*0.298*0.298*0.298*0.298)));
          $u=$u-(G*(1/$T-(1/0.298)))+(K*Math.log(($T/0.298)));
          return $u*1000;
}


/**
* This method calculates the molar entropy
 * @return double
 * @param $T double (K)
 * @param $p double (bar)
 */
public double s_gaz_mol (double $T,double $p) {

  $T=$T/1000;
double   $s=(A+8.314)*Math.log($T/0.298)+(B*($T-0.298))+(C/2.*($T*$T-(0.298*0.298)));
          $s=$s+(D/3.*($T*$T*$T-(0.298*0.298*0.298)))
          +(E/4.*($T*$T*$T*$T-(0.298*0.298*0.298*0.298)));
          $s=$s-(G/2.*(1./($T*$T)-(1./(0.298*0.298))))-(K*(1./$T-(1./0.298)));

          return $s-(8.314*Math.log($p));
}

/**
* This method calculates the complete state of an ideal gas
* (U,S,H,V,Xh,Cv) en Unités SI
 * @param p double (bar)
 * @param T double (K)
 */
public void etat_complet (double T, double p) {
          U=u_gaz_mol(T)/M ;
          S=s_gaz_mol(T,p)/M ;
          H=U+$R*(T-298)/M;
          V= $R/p*T/100/M;
          Xh=H-(S*T0_xh);
          Cv=(Cp_gaz_mol(T)-$R)/M*1000;
}

} // End of class GazIdeal
```

1.3 Assistance provided by the modeling environment

Documentation is required to use the model effectively. Increasingly, the modeling environments seek to automate the coding and especially its update. Below is an example of one that is automatically generated by the Java environment.

Method Index

- **Cp_gaz_mol**(double)
  Cette méthode calcule le Cp molaire.
- **calc_fluid_com**(int)
  Cette procédure prépare le calcul par comp_molaire des coefficients du Cv d'un mélange par application de la loi de Dalton, ainsi que M et s0, enthalpie de mélange
- **comp_molaire**(int)
  Calcul des propriétés molaires d'un gaz composé par application de la loi de Dalton
- **etat_complet**(double, double)
  Cette méthode calcule l'état complet d'un gaz idéal (U,S,H,V,Xh,Cv) en Unités SI

By activating a hyperlink, you can access more detailed documentation:

etat_complet

```
public void etat_complet(double T,
                         double p)
```

Cette méthode calcule l'état complet d'un gaz idéal (U,S,H,V,Xh,Cv) en Unités SI

Parameters:

p - double (bar)
T - double (K)

Once the class is written, its use is very simple, as shown in the following example, to calculate the differences of the values of thermodynamic functions between two points.

GazIdeal class is instantiated under the name "monGaz" and access to its public methods and variables is done by placing their name on the right of "monGaz". If the modeling environment allows, which is generally the case, all accessible elements are automatically offered to the modeler, which greatly facilitates the assembly of the models. This is shown in the following example: in the list appear the variables and methods accessible from the outside of the class.

```
public class CalculGaz
{
    double DH,DS,DU;
    CalculGaz(String nomGaz,double p1,double T1,double p2,double T2){
        GazIdeal monGaz= new GazIdeal(nomGaz, true) ;
        monGaz.etat_complet(p1, T1);
        DH=monGaz.H;
        DS=monGaz.S;
        DU=monGaz.U;
            monGaz.etat_complet(p2, T2);
        DH=DH-monG
        DS=DS-monG
        DU=DU-monG
}

}
```

```
contient_H2O
Cp_gaz_mol(double)
Cv
data
equals(Object)
etat_complet(double, double)
f_dicho(double, double, String)
fract_mass
fract_mol
gaz_existe
getClass()
```

2 THE CONCEPT OF DIGITAL MODEL

Numerical models are probably the most powerful basic tools to study complex systems. Modeling is a necessity and it does not supplant the experiment ; it is a complement which lowers the cost of studies and aloows one to understand the operation modes otherwise inaccessible to direct observation.

A numerical model is a simplified mathematical representation (or abstract approximate representation) of the studied system, which allows one to analyze its behavior. This is an operational tool that the engineer or physicist develops to solve the various problems he faces.

It should be noted that a model is false by definition. Thus, it can have behaviors that are specific, distinct from those of the system studied. On the other hand, it may fail to represent some behaviors of the system. What is important is that these approximations do not influence the interpretations we make. In this sense, there are no bad models, there are only models inadequate or improperly used.

We can define an analytical modeling based on a decomposition of the problem and the application of physical laws and an empirical modeling, based on correlations or laws derived from experimental data (especially when the complexity or randomness of the problem studied prohibits an analytical approach). In fact, the models used are often the result of a compromise between these two ways of working.

2.1 Analytical or deductive modeling

Depending on the objectives and nature of problems to solve, we will use, as appropriate, models of varying sophistication: for example, because of its greater strength, a closed loop control will be satisfied with a much simpler model than an open loop control.

Three types of analytical models can thus be defined:

• approach models, simple but possibly simplistic, are designed for a first approach of the problem by choosing a simplified modeling, "first order" for example, to get an idea of the main trends of system behavior, and identify the main parameters that govern it. However, it is not always possible to establish them a priori, at least with sufficient accuracy in practice.

• knowledge models, highly detailed but often heavy and expensive to use, are at the other end of the scale. Based on a detailed physical analysis of the phenomena involved, their advantage is the precision, but their disadvantage is the complexity and they are cumbersome to implement. Furthermore they must be validated, which can be an extremely complicated task. They are as impressive stacks of equations with many parameters among which it is difficult to discern a priori those which are most significant.

• reduced models are something of a compromise between the simplicity of implementation of approach models and accuracy of knowledge models from which they are derived algorithmically. They reflect the fact that the overall behavior of a system, however complex, may be relatively simple. Reduction procedures allow one to find the theoretical link between the laws of physics (knowledge models) and global behavior of systems (identified models).

The development of a physical model, in particular a knowledge model, involves four basic steps:

2.1.1 Analysis of physical phenomena and critical evaluation of assumptions

The transition from real-world to modeled system requires assessment and analysis of the phenomena involved This phase is important because it determines the accuracy and fineness of the model. It requires good theoretical knowledge, a systematic literature search, a minimum experience of the topic and especially a critical attitude towards the assumptions made.

Indeed, model a system requires an assessment of the magnitudes of the phenomena studied (hence the importance of the role of dimensionless numbers and their correct use) and a consistent level of complexity. The multi-disciplinarity of this phase should be emphasized.

2.1.2 Selection of the appropriate mathematical representation

Developing a knowledge model implies writing mathematical equations associated with the phenomena described, and this formal representation stems from choices made during the physics analysis phase. As discussed below, several formal mathematical representations are possible (partial or total derivatives, integral formulation...), and / or several possible discretization schemes (finite differences, finite elements...). The choice will depend on the objectives, the required accuracy and the nature of the boundary conditions. Sometimes, as we shall see about linear heat transfer, pre-processing can be performed on general mathematical formalism corresponding to the discretized equations, allowing for significant time savings for the future.

2.1.3 The choice of numerical method

When the problem has been properly stated in an appropriate mathematical formalism, it is possible to proceed with its resolution.

In most cases, the mathematical model does not admit analytical solution, and we have to resort to numerical techniques to obtain the desired results. The numerical analysis is a discipline in its own right, often poorly understood by non-specialists such as heat transfer engineers. Among the methods commonly used, we must first include the techniques for solving linear systems of the type AX = B, such as Gauss, and techniques for more general nonlinear systems (dichotomy, Newton-Ralphson...). Then there are specific methods for non-stationary problems, particularly of interest here: discretization with respect to time, consistency, convergence and stability of the discretization scheme.

Finally, when necessary, we must use methods for solving systems of differential equations (Runge Kutta ,...), or partial differential equations (method of characteristics ,...).

Increasingly, these methods use standard routines available in the math libraries, which simplifies their use. One more step is taken with the development of intelligent interfaces or expert systems that can automatically select the most suitable numerical procedures to solve a given problem.

2.1.4 The development of a computer program

Today, in almost all cases, a model is finally presented in the form of a scientific computing program constituting the computer translation of all the previous steps.

Since the 80s, the development of computational capacity and artificial intelligence languages allows us to envisage a new approach to digital tools: are emerging, in addition to numerical codes implementing the methods and algorithms known, powerful CAD type environments whose role is to break down the barriers between the formal representation of a problem and its resolution.

This has already been observed in mechanical engineering (CAD, CAM), industrial design, architecture, office automation (word processing, graphics software) and starts appearing in engineering, research and education. Recently there are scientific software environment for flexible, wide range of applications, conditions of use variables (geometry, boundary conditions ,...).

2.2 Validation of models

As noted above, a model is only an abstract representation of physical reality, and it is important to keep constantly in mind that limit. However, experience proves that, once a model has been developed, it is used very frequently. An elementary precaution, although sometimes difficult to implement, is to validate this model by comparing it to experimental results. This raises many difficulties in practice, among which two are fundamental:

• experimentation and instrumentation
• the validation procedure.

2.2.1 Experimentation and instrumentation

The primary objective of modeling being to reproduce as faithfully as possible the behavior of a real system, it is very important to be able to observe quantitatively the system, hence the crucial role of instrumentation and the difficulties related:

• the choice of sensors of sufficient accuracy and adapted to the system studied (time constants, range of validity of measures)
• knowledge of bias and systematic errors introduced by the presence of the sensor (the size of the bias between model and the measured value, uncertainty).
- The choice of numerical parameters introduced in the model (different experimental conditions, uncertain bibliography).

2.2.2 The validation process

It is not enough to have high quality experimental data to validate a model. It is also necessary that the model is sufficiently sensitive to test conditions for reliable conclusions to be obtained. For example, we know that in a transmitter traversed by heating water in forced circulation, the thermal resistance between water and the metal is very small compared to that between the metal and the ambient air. Given the inaccuracies in the second, we usually cannot get the value from the first by an experiment in real conditions, whatever good it may be.

Validating knowledge models of significant dimensions raises complex methodological problems, which are also partially confirmed by the theories of model reduction and identification, which show that given a set of inputs and outputs (experimental data), a knowledge model is far from unique.

2.3 Empirical or inductive modeling

When the complexity of the system is very high, the number of components, interactions and descriptive parameters does not always allow one to have a deductive approach. In this case, there are techniques which, from experimental data (IO) allow one to build simplified mathematical models, called behaviour.

When a deductive model is possible, this approach can give the general form of such a model (see theories of model reduction). Here we find the concepts of black box or gray box introduced by the systemic approach (see below).

This non-phenomenological modeling does not allow one to improve or optimize the system under study. However it allows one to characterize an existing system, to simulate, or to control it. The methods used are borrowed mostly from the control and statistics science (regression, correlation, identification...).

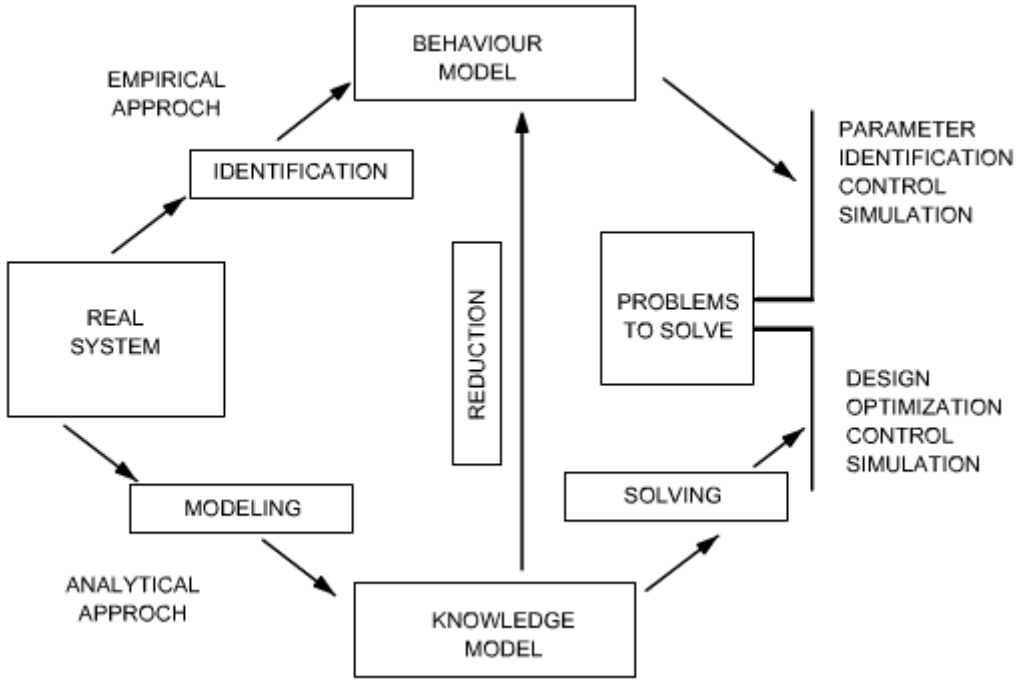
Among these, the **identification** is particularly attractive: a study of black-box type can be used by only analyzing the inputs and outputs of a system, to obtain good models, even in the absence a pre-set equation modeling based on the laws of physics. Identification methods therefore provide further insight into the traditional approach to physics. In the broadest sense, the identification phase is to determine the numerical values of parameters used in the model, the selection criterion being to minimize the error between the calculated quantities and magnitudes observed experimentally.

In a deductive approach, most of the parameters introduced in the model have a physical sense. These parameters were measured and some are known accurately, others are known in ranges of precision too large or impossible to measure. Finally, the more the model takes liberties with respect to phenomenology, the more appear parameters having no physical meaning, sometimes referred to as calibration parameters. Ultimately, in a purely inductive approach, the parameters often have no direct physical meaning.

Identification techniques are borrowed from applied mathematics (statistical techniques) and control science. To minimize the error between calculated quantities and experimental values, we use identifcation algorithms:

• online and offline identification
• gradient methods, least squares, recursive.

2.4 MODELING TECHNIQUES



In summary, to study a real system, the modeler can appeal to a variety of modeling techniques, which can be schematically represented by the figure above.

The analytical or deductive approach is to develop a knowledge model by decomposing the system into elements small enough that the laws of physics are applicable. Facilitated by the use of powerful computer interfaces, it provides a versatile but expensive tool, sometimes cumbersome to implement, used for design, optimization, control or simulation.

The empirical or inductive approach, based on the experimental overall study of the input-output behavior of the system, is to identify a synthetic model, very concise, usable for the characterization, simulation and control, but not well adapted to the optimization or design.

Between these two approaches, bridges exist, such as model reduction procedures.

These two approaches represent two extreme cases, the complete system being either broken down analytically in a very fine way, to establish a knowledge model, or globally considered to identify a behavior model.

In fact, it is quite possible to mix these two techniques and to establish a composite model where certain system components are modeled analytically and some other empirically.

Of the four stages of the deductive model we have presented only the first, and to a lesser extent the second, correspond to principal areas of expertise and interests of the modeler. The last two are necessary but are from different disciplines: numerical analysis and software engineering.

As we will see later, the current trend is to give the engineer the ability to focus on the points that constitute his field of excellence, namely the physical analysis of the phenomena and the choice of suitable mathematical formalism.

We will now explore these two points, before addressing the presentation of systems modeling techniques.

2.5 Development of physical models

In this section we will study more precisely what is usually called the development of physical models, examining the various forms of models that can be obtained, depending on assumptions.

In practice, the modeler selects the type of model to be implemented according to the objectives he pursues. His choice is the result of a realistic compromise between the fineness, i.e. the modeling accuracy and the cost of resolution, i.e. its mathematical complexity.

If one seeks to give a typology of models, it is therefore interesting to consider two additional approaches:

- The fineness of modeling, since the inclusion of corpuscular phenomena until the establishment of macroscopic balances on aggregate discrete sets.
- The mathematical form of the generated model: algebraic equations, differential or partial derivative.

The first type is used to analyze how the models fit into each other, like Russian dolls, depending on the desired fineness. They illustrate the continuity between the atomic or molecular phenomena and quantities needed by the design engineer. (It however does not allow to conclude on the desirable level of analysis).

The second type is used to classify models according to their mathematical complexity, and therefore the difficulties to be encountered during the resolution phase.

A physical model involves variables representing the state of a system, which is a priori a function of time and position of the point considered. These variables can be grouped into two broad classes:

• the **intensive variables** such as pressure, temperature, voltage, corresponding to potential functions,
• the **extensive variables** such as flow, heat flow, or entropy, intensity, which correspond to flow functions.

An intensive variable links condition in a matter point considered a reference condition to another point or another medium. For example, the temperature is defined relative to zero or the freezing point of water.

An extensive variable, however, is defined by the point considered, and is a measure of the flow through an elementary section of matter. The flow-rate in fluid mechanics is an example of such a variable.

In general, heat transfer models are set by writing the laws of continuity and conservation of extensive variables: mass, energy, and momentum, the balance being established at the control volumes of variable size.

Conservation laws written in the general form:

$$\left\{\begin{array}{l}\text{accumulation}\\ \text{in the control}\\ \text{volume}\end{array}\right\} = \left\{\begin{array}{l}\text{inward transport}\\ \text{by the}\\ \text{surface}\end{array}\right\} - \left\{\begin{array}{l}\text{outward transport}\\ \text{by the}\\ \text{surface}\end{array}\right\} + \left\{\begin{array}{l}\text{transfer}\\ \text{through}\\ \text{the surface}\end{array}\right\} + \left\{\begin{array}{l}\text{generation}\\ \text{in the}\\ \text{volume}\end{array}\right\} - \left\{\begin{array}{l}\text{consumption}\\ \text{in the}\\ \text{volume}\end{array}\right\}$$

Building a model is to translate this semantic phrase into a set of equations and set the initial and boundary conditions, then write the corresponding computer program.

2.5.1 Particle or microscopic level

The finest possible modeling today is to analyze a phenomenon at particle level. At this level, the models consider the control volume is composed of discrete elements, atoms, molecules, particles that interact according to certain laws. Global properties are obtained by summing over all particles considered.

The methods correspond to quantum mechanics, microscopic and statistical thermodynamics... Unfortunately, the mathematical complexity of the models generated is such that in practice the heating engineer rarely resorts to it. This level of analysis is therefore mentioned here only as a reminder.

2.5.2 Continuous macroscopic models

Macroscopic continuous models are established, as we shall see, on the basis of phenomenological laws, assuming that the medium studied can be considered continuous.

While in the previous analysis, we "counted" atoms or molecules, we are interested here in control volumes that, although very small, already contain significant numbers of molecules.

For example, in the normal state, a cubic micron of an ideal gas contains 2.6910^7 molecules. At the engineer scale, a cubic micron is an infinitely small control volume.

In the macroscopic analysis, writing conservation balances is made by considering a small volume element, selected from the coordinate system best suited to the geometry considered.

Most commonly, this is Cartesian, cylindrical or spherical (see figures below)

The approach is to write the balance of the volume element considered, then pass to the limit by letting the sides of the volume to 0.

As:

$$\frac{\partial f(x,y,z,t)}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x; y; z; t) - f(x;y;z;t)}{\Delta x}$$

Let: ρ density of the fluid

$V = {}^t(Vx, Vy, Vz)$ the velocity of the fluid.

The accumulation of mass in the volume is written:
$[\rho\, \Delta x\, \Delta y\, \Delta z]_{t+\Delta t} - [\rho\, \Delta x\, \Delta y\, \Delta z]_t$

The mass entering through the surface (transport):
$[Vx\, \rho\, \Delta t\, \Delta y\, \Delta z]_x + [Vy\, \rho\, \Delta t\, \Delta x\, \Delta z]_y + [Vz\, \rho\, \Delta t\, \Delta x\, \Delta y]_z$

The mass leaving through the surface (transport):
$[Vx\, \rho\, \Delta t\, \Delta y\, \Delta z]_{x+\Delta x} + [Vy\, \rho\, \Delta t\, \Delta x\, \Delta y]_{y+\Delta y} + [Vz\, \rho\, \Delta t\, \Delta x\, \Delta y]_{z+\Delta z}$

Since there is no consumption or generation term mass balance is written:

The passage to the limit provides, in the general case, a mathematical expression with partial derivatives.

For example, writing in Cartesian coordinates, the law of conservation of mass for a pure fluid gives:

$$(1)\quad \frac{[\rho]_{t+\Delta t} - [\rho]_t}{\Delta t} = \left[\frac{[\rho Vx]_x - [\rho Vx]_{x+dx}}{\Delta x} + \frac{[\rho Vy]_y - [\rho Vy]_{y+dy}}{\Delta y} + \frac{[\rho Vz]_z + [\rho Vz]_{z+\Delta z}}{\Delta z} \right]$$

By passage to the limit:

$$\frac{\partial \rho}{\partial t} = - \left[\frac{\partial (\rho Vx)}{\partial x} + \frac{\partial (\rho Vy)}{\partial y} + \frac{\partial (\rho Vz)}{\partial z} \right]$$

$$\frac{\partial \rho}{\partial t} + div(\rho \vec{V}) = 0$$

The models of thermal engineering commonly described in this form include:

• the macroscopic equations of thermodynamics, usually expressed at equilibrium,
• the equations of conduction,
• the equations of fluid mechanics (Navier-Stokes).

The advantage of this type of analysis is that it has a great descriptive power. In reality, the properties of the media studied may depend on their position in space and time: they are distributed, and only the formalism of partial differential equations allows to take them into account accurately.

Media studied in physics are always in the practice of macroscopic volume, the writing of continuous models leading to an accurate physical representation of what is happening within the mass. Knowing the boundary conditions and initial conditions, it is theoretically possible to integrate the equations, and thus have access to global variables of interest to the engineer.

In practice, however, a number of issues will arise during the integration:

First, in the example considered, we see that it is necessary to know the precise law of velocities in order to determine the density. Often, this knowledge is beyond the modeler. This is the case, for example, of a turbulent flow where the instantaneous velocities in the three directions change very quickly. At most can we get in this case access to an average speed.

Second and more importantly, partial differential equations have rarely analytical solutions and their numerical solution is complex and calculation time consuming.

The basic difficulty arises because the dimensions of the state space (spatial coordinates and time) are infinite.

In conclusion therefore, the analysis leads to very accurate models, but difficult to handle.

2.5.3 Continuous macroscopic averaged models

When one of the quantities involved in the equations cannot be determined accurately, the averaged macroscopic models, unlike the previous ones, are established by replacing this magnitude by an average value plus a zero mean disturbance. This introduction in the equations has the effect of replacing the unknown quantity by its average value, and to reveal additional terms representing the cross product of disturbances, whose average value is not zero.

A major field of application of this method is the study of turbulence, especially in fluid mechanics and convection.

The formalism that we end up here still is that of partial differential equations.

2.5.4 Averaged one-dimensional models

In many cases, analysis of the phenomenon can reveal the existence of a preferred direction of flow.

This applies, for example in a counter-flow heat exchanger in concentric tubes, where longitudinal variations of physical quantities are much larger than their radial variations.

In the averaged one-dimensional models, we neglect all changes other than that corresponding to the maximum component of the gradient. With this assumption, we greatly simplify the mathematical formalism, by keeping only one space state variable space and time. In addition, when we are only interested in steady state, the formalism is simplified further, the model becoming algebraic-differential.

Note that averaged one-dimensional models are commonly used because they often provide a good first-order problem while retaining the assumption of a continuous variation of a variable position. Many problems can be considered as a first approximation one-dimensional and lend themselves to this approach.

Let us quote for example, in fluid mechanics, the theory of one-dimensional flows, the calculation of many industrial flows (nozzles, calculation of blades, ducts...), in heat transfer, the field of forced convection and many problems of conduction.

2.5.5 Aggregate models

Often, it is not necessary (or possible) to know the inner workings of a process, even by a one-dimensional averaged method.

We can then neglect all the gradients, assuming a homogeneous mixed medium, and the studied variables become independent of the position. The independent variables are time, the quality of a phase mixture, concentrations of constituents... but considered as average values. This type of model is often called aggregate model (lumped parameters model).

This leads to macroscopic models often calibrated against experiment with theoretically impossible to calculate parameters such as global effectiveness or efficiency.

This is the case for many changes in thermodynamic compression or expansion devices, where the irreversibilities are determined through an isentropic efficiency, or by a polytropic coefficient.

This is also true of systems where one is interested in the final state regardless of the transients.

2.6 Classification according to the mathematical form

2.6.1 Mathematical formalism obtained

Physical models include three types of equations in order of complexity:

• algebraic
• ordinary differential (ODE)
• partial derivative (PDE).

Algebraic equations do not contain any derivative form by definition. They can be used to represent spatial and temporal continuous variables. Models using these equations correspond, in the typology above, to aggregate models in steady state.

In an ordinary differential equation, there is only one independent variable that varies continuously. It is therefore limited either to a single space variable or a change in time.

The first case is that of one-dimensional steady state averaged models, the second that of the aggregate transient models. These two cases represent in fact already a wide variety of applications. As the mathematical treatment of systems complexity is much lower than that of EDPs, models of this type are often used.

The value of partial differential equations is that, we have seen, they correspond to the natural formalism in which the engineer describes his physical models in continuous media.

Two, three, four independent variables can be considered simultaneously in the modeling. In most cases, time is at least one of the independent variables and the number of others depends on the geometry considered. The use of cylindrical or spherical coordinates reduces the number of spatial variables in case of symmetry.

The main drawback of the EDP is that their solution is all the more complex than the number of independent variables is large.

A trick is thus to discretize the space to replace the continuous medium by the juxtaposition of finite volumes and write for each volume balance equations, by keeping only one term derivative, for example time. If the selected volume is small enough so that it can be considered homogeneous, one replaces the resolution of a single EDP by that of a large number of ODEs. These methods (finite differences, finite volumes) are very commonly used, especially to study the transient one-dimensional models.

2.6.2 Selection criteria for modeling

When we wish to model a system or component, we always try to achieve a specified goal (s). The explanation of this (these) objective (s) is a fundamental step in modeling, that strongly influences the basic choices, particularly concerning the mathematical formalism used.

1) Partial Differential Equations

In addition to help conserve natural formalism for writing balances in continuous media, the EDP provides access to position variables in the medium. In this sense, they are used to study the fine geometric characteristics of the components studied.

The field of application of models that use them is that of the geometric design of complex parts (detection of maximum stress areas, hot spots studies, study of flows, route profiles ...).

Their disadvantage is that solving methods are cumbersome and difficult to handle, and are not always justified.

2) Ordinary differential equations

Models using ODEs are usually simplified versions of the previous ones: dynamic aggregate models, one-dimensional static models.

Simplified, these models are often less "natural" because truncated due to various assumptions, implicit or explicit. Their main advantage is that the simplifications made generally make them much more manageable than the distributed parameter models.

In particular, it is almost always possible to linearize around an equilibrium point or for a limited range of variation, in which case we have a considerable mathematical apparatus for studying the phenomenon in question: internal description by linear modal analysis, external description by transfer functions, stability study, criteria for controllability and observability, identification of model parameters...

The introduction of boundary conditions for the transient study of systems is suitable, in the case of ODEs, to a relatively simple formalism of coupling of components models and defining a vector of loads exciting the system.

In addition, it is relatively easy to take into account changes in structure of the system considered by coupling a controller to the set of differential-algebraic equations.

As techniques for solving ODEs are much more developed than those of PDEs, there are solvers capable of solving in excellent conditions models with hundreds of equations with discontinuities.

Another point to consider is that there are often relatively clear links between the ODE physical models and models obtained by the empirical approach methods. In some cases, these links can be explained within the framework of a theory of model reduction, and give rise to specific algorithmic procedures (linear thermal models for example).

In other cases, they simply stem from the similarity of assumptions implicitly or explicitly adopted in the development of models.

For all these reasons, the models represented by differential-algebraic systems are now widely used in the field of engineering science and the art of the modeler is often to find the sound assumptions for transforming a PDE model in ODE.

In conclusion, the ODE formalism corresponds to an extremely broad model field, for which we have proven analytical tools. In particular it is probably best suited to the study of interconnected systems with discontinuities, as it allows to analyze the stability, observability and control.

However, the ODE models are less suitable as PDE models for the precise definition of the geometry of system parts or components.

The two types of formalism thus appear complementary and the choice between them will be made according to the objectives of the modeler.

3 SYSTEMIC APPROACH

The notion of system has appeared there is less than 50 years as a common denominator in disciplines as diverse as economics, energy, biology, sociology, to better understand the organized complexity.

In fact, this new discipline was born from the limits of conventional Cartesian method, the dominant paradigm in Western science, which is still well suited to the analysis of branching processes, even complex, but whose formalism does not address in good conditions the study of large systems strongly coupled, where one cannot isolate "parts" soluble regardless of the whole.

3.1 Cartesian approach and systems approach

The limits of the Cartesian approach is all the more clear that we are interested in complex and organized systems, purposeful and able to evolve and adapt autonomously.

Knowledge of the laws of behavior of the fundamental elements of the system is not actually needed to understand the behavior of the whole, that is not reducible to the sum of its parts: human beings cannot be reduced to a sum of organs and skeleton...

To understand the organized complexity, systemic approach focuses on the functions, relationships, feedback loops, memory, self-tuning... all concepts which are more and more used in the vocabulary, but still lack a general universally recognized conceptual framework.

Le discours de la méthode de Descartes, fondement de la démarche scientifique classique, est basé sur quatre préceptes fondamentaux remis en cause par les systémiciens :

Descartes speech of the method, the conventional scientific basis, is based on four tenets challenged by systemists:

Precept of evidence

"The first [is] never to accept anything as true that I do not [know] of course, be such, that is to say, carefully to avoid precipitation and prejudice, and not understand anything more in my judgments than what appears [this] so clearly and distinctly to my mind that I [have] no opportunity to question it. "

This precept calls for two comments:

• first, the subjectivity of the concept of evidence. As the history of science and thought has abundantly shown, several proclaimed truths have subsequently been challenged and eventually be abandoned ...

• secondly, we sometimes deal with problems not obvious but crucial, that the first precept of Descartes would tend to dismiss for lack of clarity and obviousness.

Against this precept of evidence, systemicists oppose the principle of relevance: it is in relation to explicit purpose that our intelligence is exercised. A concept will be relevant if it is operating, not if it is evident in the absolute.

Precept of decomposition

"The second, to divide each of the difficulties I [consider] in as many parts as [is] possible and [is] required to better resolve."

Behind this precept, so unanimously accepted, lies a major challenge: Descartes does not explain how the division should be done, and inappropriate division may increase the difficulty of the problem ...

At this top-down approach, the systemic approach tends to combine a bottom-up approach, starting from the parts and leading to the whole, open on the system environment...

Precept of causality

"The third, to conduct my thoughts in order, starting with the simplest and easiest to know objects, to go up gradually as if by degrees, to the knowledge of the compounds, and even assuming an order between those that do not naturally precede one another. "

This causal precept is also the base of much of Western thinking. Valid for simple systems according to deterministic laws, however, it is void for advanced systems that could break the causal chain to achieve their goals.

The failure of many forecast models based on the extrapolation of the "laws of the past" is there to testify.

To the causal precept, the systemic approach opposes the teleological principle that makes thinking about the purpose of the object under investigation one of the keys to understanding it.

As the top-down approach closely allied to the precept causal, the bottom-up open on the environment approach is closely associated to the reflection on the goals, as illustrated by the scope of the concept of systems with goals, adapting and innovating to meet their goals

Precept of completeness

"And the last, to do everywhere enumerations so complete and reviews so general that I [am] sure to omit nothing."

In fact, the fourth precept was often put in default because ... impractical ... in practice.

Aware of the impossibility of meeting the latter obligation, the systemicists prefer an agregativity principle, linked to the principle of relevance, that any representation being necessarily subjective, it is more important to find the rules for selecting a relevant way the aggregates to be considered, rather than have illusions about the objectivity of a relevant survey.

We see, in a foundation burst, systems thinking school seeks to stand firmly of Cartesianism. Without doubt this is all the more necessary that the objective being to approach the study of large organized systems (biological, social, ecosystems...), it is clear that the dominant Western way of thinking does not completely master.

3.2 Complementarity of the two approaches for the study of physical systems

For what interests us, namely the technical systems programmed and even self-adapatative, it seems that there is actually more complementary than opposition.

So we will try to benefit from the insights that each way of thinking can provide, hoping to show a stereoscopic image more easily accessible to our understanding.

Drawing on concepts such as negative-feedback, memory, self-tuning, the systems approach has the ambition to offer a general key to understanding to better manage complex systems, to apprehend them in whole, by providing access to their fundamental invariants, their main determinants, which are beyond the traditional analytical approach.

At the microscopic view provided by the latter, which seeks to bring a system to its simplest components in great detail, but at the cost of losing the big picture, the systemic approach gives a macroscopic view that accepts a blur in the details, but provides an understanding of the overall behavior.

For many years, these two approaches were considered mutually exclusive. The systemicists were satisfied with a rough description of elementary phenomena, arguing, often rightly, that their goal did not require analytical precision, which led to modes of representation too heavy to be used in practice. Analysts, meanwhile, refused to give confidence to the results provided by the models they considered wrong according to their criteria.

In fact, some evidence suggests that this cut is likely to evolve in the short term, as analytical approach and systems approach can be reconciled more and more frequently, with one hand the use of powerful computer-assisted analytical techniques, and also the development of methods to reduce algorithmically complex models, to demonstrate for a particular purpose, behaviour models concise but very precise.

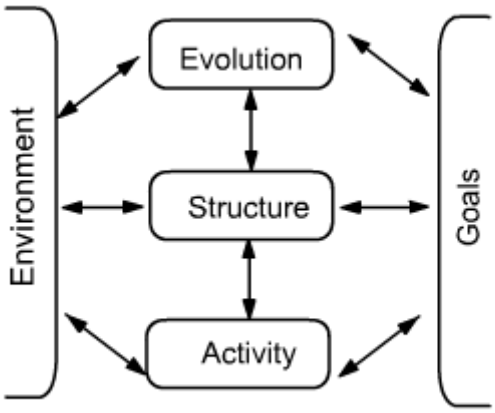
3.3 Principles of systems modeling

Introducing a systems modeling approach is even less easy as it is an evolving theory, which still lacks a universally recognized theoretical framework. One of the best summaries is probably the General System Theory of J. L. Le Moigne (1984), which defines itself as a systems modeling theory, to which the interested reader may refer.

A special feature of this presentation is to build an artificial General System, having all core systems characteristics. It is a sort of a model of models, which provides an analytical framework for all real systems, whose main interest is to provide guidance for operational modeling.

3.3.1 The General System Theory

Any a priori definition of a system being either too restrictive or too vague to be operational, J. L. Le Moigne defines it from the description of the following figure:



A system is "an object in an environment with a purpose, which carries on activities and sees its internal structure change over time, yet without losing its unique identity"
or:

"An active object)
and stable)
and evolving)
in an environment,
and in relation to some purpose. "

The theory of General System's objective is to describe the general system with the "permanent features associated with the conjunction" of these five concepts.

The General System will then constitute a fundamental reference for the modeler who, when he has to build the model of an existing or proposed system, will ensure that this model is isomorphic to the GS (and of course homomorphic to the real system).

3.3.2 Basic Concepts of the General System

• Activity of the General System

While in the development phase of physical models, emphasis was placed on the analytical description of the phenomenological laws, the activity of System General will focus, in the spirit of the systems approach, on functions of elements studied.

a) The processes

One of the basic concepts to describe the GS is the process, incorporating the concept of elapsed time, and depicting "any change in time of matter, energy or information."

A **processor** will move a "processed" object in a 3-D TSF reference: time, space, form. It represents well the function (s) of a system component.

Specific processors can be limited to a change in time (T processors such as storage, memory) in space (S processors such as transport, communication) or in form (F processors such as transformers). The most general ones effect change in the three directions at once.

Very typically, there are three major categories among the "processed" objects, **matter, energy and information**. The mathematical description of their evolution will use the notion of state variables, *essentially the intensive and extensive variables studied above*.

	Processor types	
	matter-energy	**information**
S Processors	ingestor injector dealer extruder extractor	driver receiver channel transmitter
T Processors	storekeeper shopper accumulator	memory replicator
F Processors	destructor producer filter catalyst	decoder encoder calculator regulator

More precisely, we differentiate among information flows, the control signals (orders), other (data) (see table). These information flows will be important to observe and control the system. *They are the basis for the construction of automated control*.

b) The black box

To describe a process, the analytical approach uses classical writing of all relationships that explain its internal behavior. A purely functional approach does not necessarily have that luxury details. Where it is possible to establish a pattern of behavior based on the analysis of but the process I / O, without any assumptions about its physical content or abstract, it is called a "black box" model. This concept has proven very powerful, especially in control science, where often it is not necessary to know the process from the inside to control it. *The link between the notion of black box and the models presented above is immediate*.

In this representation, the variables associated with inputs and outputs are called coupling variables. The causal link between outputs and inputs is the distinction between dependent and independent variables.

c) The gray box

In some cases, we know the content of part of the process, or its structure. It then becomes possible to establish more accurate models or of a wider range of validity by using this information to guide the model choice.

This is called a "gray box" model. *This notion, which is very vague, is roughly in physics aggregated models as have been defined above*.

• Structure of the General System: a network of elementary bounded processors

Having established a set of concepts for describing the functionality of components, taking into account the whole system is done through the study of its structure and its evolution.

One of the fundamental assumptions of the GS is that it consists of a set of active elements, each following a specific constitutive law, or of elementary processors, which can be either T, S or F. This distinction should not be made too narrowly. In some cases, We will make use of multi processors, reduced to the previous decomposition. Each processor may, without prejudice to the way it is described or modeled, be represented by a box (black, gray or otherwise), equipped with one or more inputs and one or more outputs.

The GS is then constructed as a combination of multiple processors. The set of connections linking the input and output basic processors form its inter-network, whose topology is a fundamental characteristic of the GS.

Matrix or graphical representations of the network can be established, showing connections between the inputs of the various boxes representing the processors and their outputs.

It should be noted that to a very large extent, the structure of a system is independent of the level of fineness of the modeling (box contents). *This organizational structure characteristic of the system under consideration may therefore be subject to specific tests that remain valid if some process models are changed. This property allows one to operate in an iterative manner, while maintaining the gains of the previous phases, which is very efficient and economical*.

The general topology of the network itself is representative of the complexity of the system under consideration. Two major types of relationships are of paramount importance: the trees, and feedback.

The appearance of the second type is relatively new and is to the credit of cybernetics, which first introduced and developed the concept of feedback, of major importance in control science.

It can be shown that the levels of complexity associated with network feedbacks are of a higher order than for tree networks. The "feedback degree" is representative of the complexity of a system.

. Decomposition of the General System

Two of the main tasks of the systems modeler are:

• the identification of elementary processors
• the establishment of their network of relationships.

To accomplish the first task, the modeler must be able to separate the entire system by judicious choice of the points of separation, the "natural joints" of the system and the coupling variables. This act has a high level of subjectivity and explains that a given system can be modeled in several different ways, including by the same modeler.

To guide the modeler, a number of levels (nine) were attributed to the development of the General System.

• The **first level** is that of the passive object to which no need is assigned. It has no particular interest for our purposes, the passivity of the object making it unnecessary modeling it.

• The **second level** is that of the active object, stable over time, such as a simple converter, such as electrical resistance, a boiler or a turbine.

• the emergence of regulation is characteristic of the **third level**. Consider for example a Watt ball regulator, limiting the pressure of a steam boiler according to the speed of the motor shaft. This is a mechanical control at this stage, no separate circuit information.

• The **fourth level** marks the emergence of the information in the representation of the object. The relatively new idea to differentiate information signals from other objects processes, has been extremely fruitful because of the development of information processing techniques (control, scientific computing, expert systems). At the fourth level, the information is still treated summarily, either analog or digitally: *0/1 or proportional control, such as a heating thermostat*.

• The **fifth level** is the appearance of the decision, and thus, implicitly, of goals. This new feature implies the existence of an internal logic allowing the processor to choose among several possibilities, and decide, based on the values of inputs, what action should be taken. *A heating control with no memory of outside temperature is an example of such a processor*.

• In the **sixth level**, the active object has a memory, which allows it to reach higher levels of complexity. The existence of a memory allows the processor to integrate the past, and thus opens a new field of possibilities. *In terms of regulation, this field covers most of the memory PLC, since derivative and integral regulators to optimal control systems*.

• In the **seventh level**, it coordinates, structuring exchanges between the operational, informational and decision-making levels.

• In the **eighth level**, the imagination emerges and thus the capacity of self-organization. In terms of regulation, for example, the eighth level sees the appearance of concepts such as self-tuning, where the system has a learning processor that allows it to adjust at best according to the environment in which it is immersed. Expert or pattern recognition systems also belong to this category.

• The **last level** is the auto-completion, which does not yet include the technical systems.

It is clear that the modeling of physical systems does not require the inclusion of all these levels, with sometimes vague limits. In practice, the first five or six are sufficient in most cases. Moreover, it is almost always possible to separate models of high level in sub-models using lower level representations. We can thus choose models of different levels depending on our objectives.

• Development of the General System: Memory and Program

We have seen that the there is a hierarchy of processed object: matter, energy, information. For processing matter, it takes energy, for processing energy, it takes information.

While, until now, by analyzing its structure, we considered a representation of the GS where these three categories were treated in parallel, it may be necessary to differentiate their modes of representation. For the study of large high-level systems the concept of information flow (with a shade between the informational and decision-making signals) is so important that the very specific concepts of memory and program prove to be very powerful analysis tools.

As soon as systems must respond by taking into account not only the environment at the given time, but also the chronicle of past events, it is necessary to have sophisticated decision-making processors and memory, memory and programs.

A complementary notion very fruitful in practice is that of state, already discussed above, which in a sense of the term control science, represents "the minimum memory of the past needed to determine the future behavior of the system." The power of this concept is that when you can write the equation of state of a system or process, you the get a behaviour model allowing you to determine trends with great accuracy, and usually a great economy of means.

The state of a system being stored, decision-making processes become able to anticipate possible changes of the whole in response to changes in the environment.

If the system is **controllable**, it will be possible to bring it "voluntarily" in a state S (t) desired from the state S (t_0) where it is.

If it is **observable**, we are able, knowing the state at time t and the chronicle of controls and loads, go back to the different previous states.

The study of the observability and controllability of processes and systems is of particular importance for defining their control.

More generally this formalism allows you to address the problems associated with changes in the active structure discussed above.

. Environment and goals

The General System Theory has not yet formalized the nature of the links that connect the GS to the environment or the problem of purpose. This last point, which applies only to systems with high-level goals, is somewhat foreign to our purpose, and will not be dealt with. The first gap is a bit worrying in that the boundary conditions of any system have, as we know, a key role on its behavior. *That is, as stated in the study of ODE or PDE equations, there are mathematical techniques for consideration in the case of physical systems.*

4 MODELING ENVIRONMENTS

4.1 Structure of the modeling approach

The study of the concept of system has highlighted the fundamental importance of the processors and links between them. To a large extent, determine the model of a system is:

• identify and model the elementary processors or components,
• link them.

Solve the model, is to use it to get answers to problems that arise, namely design, control and characterization. In most cases, simulation will be used, which allows to study the reactions of the system when the environment changes. We must construct a simulation model, or simulator, which, given the complexity of relationships to handle, is almost always in the form of a computer program.

To achieve this, even for simple systems, we are led, as we have seen, to intervene in four complementary levels: the physical analysis of the system, the translation of mathematical laws of physics, the search of a numerical algorithm, computer programming .

Modeling complex systems is the ability to conduct all these operations in a coherent and effective manner for various processors and the network of their interrelations. In practice, it is actually common for all four steps above to be conducted in a nested way, without appearing separated. The modeler then works in parallel, using the synthetic environment as a support to assemble the various components of the system. He then defines prematurely a framework for his model, even before the analysis of all components is sufficiently advanced.

The result is a heterogeneous model in the levels of accuracy, specific for the desired application, and unreliable. Inconsistencies are frequently masked and its development is therefore complicated. In most cases, even when

its designer, by passing the time succeeds in making it run, the program developed is so specific that no one else can use it to generalize or as a basis for another model. If the designer goes, sometimes it is better to start from scratch...

This way of working, a caricature, is an unfortunate reality for many designers. The basic reason is that on the one hand, modeling is a new discipline that many people have learned on the job, and so few are aware of the importance to clearly distinguish the various steps mentioned above and secondly it is difficult to ask the person to excel both in analysis of physical phenomena, mathematics, numerical analysis and computer skills.

After an initial period, a little anarchic, during which, with the faults we have mentioned, engineers have spent many years developing their own tools from scratch to solve their problems, there has been for some years awareness of the need to operate more intelligently, in order to avoid a distortion between the time spent on computer solving techniques and that devoted to the physical or technique analysis itself.

We thus understand the importance of a structured and consistent modeling approach, applied from the level of elementary processors to that of the entire system.

The modeling environments are tools to juggle in the best conditions with all these tasks.

4.2 The numerical solvers

Proceed with caution in the development of a model, it is also to separate the most clearly possible the respective fields of modeling, numerical analysis and computer solving.

As the objects handled by the former (the physicist or engineer) result in relatively typed mathematical representations (partial differential equations, differential-algebraic systems, logic equations), it gradually became justified, whenever possible, to develop general tools to ensure numerical and computer tasks.

The use of these solvers provides a number of benefits that we examine.

4.2.1 The automatic resolution

As its name suggests, the primary function of the solver is to solve the set of equations automatically submitted to it without the user having to know the details of the resolution mode selected. Representing commonly investment of tens of man-years, these programs offer proven, solid solution to many problems. It may however happen that arise instabilities or convergence problems. The most advanced solvers provide at least in this case valuable information about these difficulties.

4.2.2 Time (and cost) significant savings

Two figures will highlight the significant time savings which provides the use of solvers. Consider that, in general, the development of a resolution programs leads him to write about 25 lines of 'source' code by equation, and that a good programmer developing programs to be maintained in good conditions has a daily productivity of 10 lines of code - development included. With two equations processed by a programmer in a week, the interest of the solvers is unmistakable. Once the physical analysis is performed to model the system, the time needed to resolve is a matter of days when you have a good solver, instead of months otherwise.

4.2.3 An open, scalable and communicable environment

The third benefit offered by modern solvers is to provide a particularly open environment. Their input language requiring a minimum of rigor in the description of the models, it is much easier to communicate with other modelers or, where appropriate, other modeling environments. The structure of the description being standardized model maintenance is facilitated, and the whole is well suited to create libraries for fruitful discussions and, gradually, the study of more complex systems. When the solver can be connected to a modeler allowing easy handling of descriptive models, the use of the solver is possible without having to know in detail the syntax of its input language.

4.3 A different path: the specific tools

The method previously discussed allows one to address in very good conditions the study of complex systems of any kind. Very generally, it has the advantage of being implemented without major difficulties, provided we have the corresponding software. That said, it does not always make the most of the intrinsic properties of the studied system, if any, and therefore masks some features that can be very meaningful to the engineer.

In some cases, especially when you have to work long with the same class of systems, it can, despite the remarks made above, be interesting to develop specific methods taking full advantage of the properties of this class of systems.

A second approach is therefore to exploit at best the mathematical properties of the formalism corresponding to the model equations. For dynamic systems, the use of theoretical body developed in the context of control science makes it possible to directly obtain very general results, with minimal need for numerical simulation. The linear heat transfer, the contribution of modal analysis and model reduction techniques show the richness of this second approach.

The Thermoptim software (http://www.thermoptim.org) shows an example of modeling environment suitable for the study of complex energy systems combining systems and analytical approaches.

CONCLUSION

Compte tenu de la complexité des phénomènes en jeu, et du degré de précision demandé, le niveau de sophistication de ces outils informatiques ne cesse d'augmenter. Deux possibilités se présentent alors à l'ingénieur : soit développer lui-même les modèles dont il a besoin, soit utiliser des logiciels polyvalents existants.

Numerical models are powerful tools to help the design engineer to mobilize his scientific knowledge to solve problems that he faces:

• design new devices, with the aim to optimize the design,
• control designed or existing systems
• describe components or subsystems.

The human brain alone no longer being sufficient to optimize the design of a dynamic system subject to multiple loads, or adjust a behavior model on the basis of thousands of experimental data, the use of computer modeling environments is becoming more and more a necessity.

Given the complexity of the phenomena involved and the degree of precision required, the level of sophistication of these tools is increasing. Two possibilities present themselves when the engineer: either developing himself models he needs, or use existing software.

The first attitude was until a few years ago the rule. As long as models were not too complex, it could indeed seem more interesting to develop them by oneself. However, over time, it appeared that create ex nihilo the precise computer model of a complex system is actually an extremely difficult task, under a series of sophisticated processes. Today it is a matter for specialists, requiring a vast knowledge in model construction technique and knowledge of basic phenomenological laws, otherwise the final product is necessarily limited, either in scope and the possibility of evolution or in accuracy and precision. In addition, it is a long and expensive task, which is justified only insofar as the specialized model that we develop is required to be used many times.

For the physicist or engineer who cannot, without exception, due to lack of expertise and time required, develop himself the range of conceptual tools they need, the second option seems more attractive: make use of general software for quick response to problems that arise. Various classes of such software already exist, and their numbers multiply: specific model to a type of application (heat exchangers, heat transfer in space, in buildings...), general numerical solvers (finite elements, algebraic-differential systems...).

A constraint still common, in addition to the cost of access, is that the modeler should describe the problem in the formalism of the host software, and often the interface between different software is tricky. To overcome

these difficulties are emerging modeling environments that allow the engineer to describe his problem in his usual language, an intelligent interface undertaking to translate the description in the formalism of the solver.

Combining the methods of classical analytical approach in terms of their basic models, and the contribution of the systems approach for the assembly of these modules to describe complex projects, these modeling environments allow him to effectively mobilize the scientific knowledge available.

However, he should not discharge his responsibilities by giving undue reliance on these tools. He must know the limits and retain a critical look at the results he gets. In addition, in all cases, a rigorous analytical approach to the problem is necessary, and a solid general knowledge in several areas is desirable:

• analytical modeling techniques, from writing phenomenological laws to choice of numerical methods, through the selection of the appropriate mathematical formalism.
• signal processing techniques, including all matters relating to the identification of models, spectral analysis and filtering.
• the basic concepts of the analysis of complex systems, that is to say, the systems approach, which is a way of thinking is particularly well suited to the class of problems to be addressed.
• more generally, mathematics applied to the physics of dynamical systems, to understand the possibilities and limits of the range of tools to be used

REFERENCES

[1] DESCARTES R., Discours de la Méthode, Oeuvres Complètes, Bibliothèque de la Pléiade, 1952

[2] LE MOIGNE J. L., Théorie du Système Général, PUF, 1984

[3] ROSNAY de J., Le Macroscope : vers une vision globale, Seuil, 1975

[4] HIMMELBLAU D., BISCHOFF D., Process Analysis and Simulation - Deterministic Systems, Wiley and Sons, NY, 1968

[5] SPRIET J., VANSTEENKISTE G., Computer aided Modelling and Simulation, Academic Press, Londres, 1982

[6] WELLSTEAD P., Introduction to Physical System Modelling, Academic Press, London 1979

[7] ROSENBERG R., KARNOPP D., Introduction to physical system dynamics, Mc Graw Hill

[8] GICQUEL R., Systèmes Energétiques, Tomes 1 et 2, Presses de l'Ecole des Mines de Paris, 2001

[9] GICQUEL, Renaud Approche systémique et thermique instationnaire. In Actes de la Rencontre SFT 92 : Colloque de Thermique "Systèmes Thermiques Instationnaires", Sophia Antipolis, France, 20-21 mai 1992. Co-édité par la SFT et l'Ecole des Mines de Paris (ISBN 2-9504471-4-7), janvier 1993, p. 337-355.