Lecture 3: Models and measurements for thermal systems, types of inverse problems

D. Maillet[1], D. Petit[2], J.-L Battaglia[3]

[1] LEMTA, Université de Lorraine & CNRS, Vandoeuvre-lès-Nancy, France
E-mail: denis.maillet@ensem.inpl-nancy.fr
[2] Institut P', CNRS UPR 3346, Poitiers, France
E-mail: daniel.petit@let.ensma.fr
[3] Laboratory I2M, Departement TREFLE, Université Bordeaux 1 & CNRS, ENSAM, Bordeaux, France
E-mail: jean-luc.battaglia@trefle.u-bordeaux.fr

Abstract. Models that can be used for later inversion, of measurements for example, are presented and classified. They fall in the white, grey or black box categories. The quantities they are based on are introduced and great care is given to the notation, in order to be able to understand the different causes of errors in the subsequent inversion output. The specific case of heat transfer is considered and the different types of inverse problems are presented. The notions of discretization of the observations and of parameterization of the functions that have to be retrieved through inversion are introduced. Reduction of a multidimensional heat transfer problem is presented by introduction of models of lower space dimensions: it allows some kind of regularization prior to any inversion. Lectures 9 and 10 will show how to get a good inversion, with the help of the points studied in the lectures in between.

1. Introduction

Modelling constitutes a very general activity in engineering. A system can be considered as modelled if its behaviour or its response to a given excitation can be predicted. So prediction is one of the natural characteristics of modelling.

Another very important feature of a model (in heat transfer or in any other field), which is only a theoretical representation of the physical reality in the case of a material system, is its *structure* (we do not deal here with information systems). In heat transfer, the choice is quite large and the model structure should be selected according to the *objective* of the model-builder.

The model-builder can have in mind an optimal design problem, a parameter estimation problem using measurements, a control problem to define the best excitation shape for a given desired output, or a model reduction or a model identification problem, just to quote a few applications.

The choice of the structure of a model in heat transfer depends on many things:

- **State variables and observed quantities**

In a heat diffusion problem, temperature is the quantity that constitutes the state variable, in the thermodynamics sense. In order to calculate temperature and fluxes at any time *t* and at any point P, one has to know the initial temperature field (at time *t* = 0) at the local scale, as well as the history of the different thermal disturbances between times 0 to *t*.

So, one has to define what is a *local* point P and a local scale. For instance, if heat transfer is intented to be studied at the very small scale in a metal, Fourier's law, relating heat flux to temperature gradient, may no longer be valid. In such a case two temperatures (respectively for the electron gas and the lattice) are required to describe heat transfer at this scale [1, chapter 1]. Such a *detailed* state model will be necessary if *observations* or predictions are looked for at the nano scale or at the picosecond time scale. The upper thresholds of both scales depend on the considered material.

We will consider, in the next sections, the case of physical systems where heat transfer takes place. So, we will make two asumptions :

- a temperature, as well as a temperature gradient, can be defined, which means that the medium under study can be given a continuous description, and
- the Fourier law linking the local heat flux and the temperature gradient is valid. This asumption is justified for time and space scales that are not too small: typically, for times larger than 10^{-11} s and lengths larger than 10^{-8} m. This corresponds to what is called a *mesoscopic* description of a thermal system.

However, even with such a system, special attention has to be taken for the definition of a local temperature for heterogeneous materials (porous media, composite materials, ...) that is all media where two phases are present at the local scale: the concept of homogenization through macroscopic homogenization has to be considered. This topic, that leads to a space filtering, has to be used at the macroscopic scale [5].

- **State definition**

The continuous state equations have then to be defined for the modeling problem at stake: it can be a partial differential equation, the heat equation (state = temperature), or an integro-differential equation, the radiative transfer equation (state = radiative intensity), or both coupled equations. Their solution, that is constituted by both temperature and intensity fields in the third case, should be calculated everywhere and any time past the initial time. It can also be a differential equation, or a system of differential equations for lumped systems where only space averaged quantities are used (an average temperature instead of local temperatures, heat flow rates instead of local heat fluxes).

Everytime state equations, based on conservation equations are used, one deals with *internal representation* and it is possible to talk of models of the *white box* type. These conservation equations are associated with constitutive laws (Fourier's, Fick's, Ohm's, Darcy's or rheological laws, ...) corresponding to the considered quantity (heat, species, electrical charge, momentum in porous matrerial or in fluid mechanics).

- **Quantities of the direct problem**

  We focus here on the diffusion heat equation in a medium composed of one or several homogeneous materials, with its associated initial, boundary and interface equations. Its solution, the state variable, here the continuous temperature field $T(t, \mathrm{P})$, has first to be found and the desired *observed quantities*, that is the (theoretical) output of the model at a given point P, $y_{mo}(t) = T(t, \mathrm{P})$, has to be calculated next.

  The quantities that are required for solving the *direct problem* are the *structural parameters* of the system (conductivities, volumetric heat capacities, heat exchange coefficients, emissivities of walls,...), the *thermal excitation* and the *initial temperature field* $T(t=0, \mathrm{P})$. Let us note here that it is possible to make a *physical reduction* of a model based on the three dimensional (3D) transient heat equation to get simpler models of lower dimensionality. The thermal fin (1D) or the bulk temperature representation (0D) constitute such reduced models. This type of reduction may also reduce the number of parameters defining the excitations.

- **Numerical/analytical models**

  There are many ways for solving the heat equation and finding a *state model* for the observations: *analytical solutions* provide the temperature field explicitely as a function of the structural parameters of the system, the excitation and the initial state. They can be constructed if the heat equation in each material and the associated conditions are all linear and the corresponding geometry simple. The other class of state models rely on *numerical solution* of the heat equation: one can quote the nodal, boundary element, finite elements and finite volumes methods, for example. State models rely on an internal representation of the system: the temperature field has to be found first and the observations are calculated next.

- **Internal/external representation**

  The models based on state equations, which are described above, corespond to an internal representation of the system: they are of the ***white box*** type and their structural parameters (thermophysical or optical properties, geometrical quantities associated to the shape or material structure of the physical system) have an *intrinsic* character since their definition does not depend on the *structure* that is chosen for the model.

  External representations, that short circuit the state variable and link directly the observation(s) to the excitation(s), constitute another class of models.

  They can be of the ***grey box*** type if the structure of the corresponding model is imposed by the nature of the governing equations: if the relationship between observed quantities (output) and stimulations (input) is linear, for physical reasons, the structure of the model is imposed and its structural parameters are the coefficients of a matrix once the input discretized and the output parameterized (see below). If, furthermore, the physical structure of the material system does not vary neither with time nor with temperature, this linear relationship becomes a convolution product and a transfer function can be defined. In that last case the model can be represented

using the *parametric approach* presented in lecture L8 “Experimental modelling through identification of low order models” of this advanced Metti school.

Another type of model of the grey box model is used in the case of thermal radiation in an enclosed cavity with opaque walls, where radiative fluxes depend on the diferences of the fourth powers of the wall temperatures.

If no information whatsoever is available on the nature of the relationship between input and output, ***black box*** models, that link observations to inputs and ad’hoc parameters (the structure of the model) has to be found. Models of this nature can be neuronal networks (multidimensional abacus), stochastic models, ...

- **Parameterization for inverse problem solution**

  Parameterization of the data of the direct problem constitutes another characteristic of the structure of a model: structural parameters, thermal excitations, and the initial temperature field are, in the very general case, functions of different explanatory variables: space, time, temperature. The conversion of functions into vectors of finite dimensions does not pose much problem in the *direct problem* (calculation of the observations, the model output, as a function of the input). It is no more the case when the *inverse problem* is considered. This point will be discussed in section 2.3.2 and in lecture 9 of this school. One of the objectives of *mathematical reduction* methods is to construct a *reduced model* that will have a reduced number of structural parameters, starting from a *detailed reference model*, see [1, chapter 13] for details on model reduction, while *physical reduction* also change the definitions of both output and excitations, see section 3.2.

2. Physical system, model, direct and inverse problems

2.1 Fourier’s law: a reminder

We will consider now on, in the presentation of inverse problems in heat transfer and in the remaining part of this lecture, the generic case of heat diffusion in an isotropic or anitropic material that verifies the heat equation. This conservation law is based on Fourier's law, where the local heat flux is defined by :

$$\vec{\boldsymbol{q}} = -k \ \overrightarrow{\text{grad}}\,(T) \qquad \text{(isotropic case)}$$

or (3.1)

$$\vec{\boldsymbol{q}} = -\bar{\bar{\boldsymbol{k}}}\ \text{grad}\,T \quad \text{with} \quad \bar{\bar{k}} = \begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ & k_{yy} & k_{yz} \\ sym. & & k_{zz} \end{bmatrix} \qquad \text{(anisotropic case)}$$

where operator $\overrightarrow{\text{grad}}\,(T)\ (\partial T/\partial x,\ \partial T/\partial y, \partial T/\partial z)$ denotes the gradient of temperature and k the thermal conductivity of the material. A symmetric conductivity tensor $\bar{\bar{k}}$ has to be

used in many cases encountered in nature or in man-made objects (composite materials for example), because conductivity is no longer isotropic but orthotropic, or more generally, anisotropic. In the principal axes of this tensor, the Fourier's law becomes:

$$\vec{\boldsymbol{q}} = - \left(k_x \frac{\partial T}{\partial x} \vec{\boldsymbol{x}} + k_y \frac{\partial T}{\partial y} \vec{\boldsymbol{y}} + k_z \frac{\partial T}{\partial z} \vec{\boldsymbol{z}} \right) \tag{3.2}$$

The (continuous) material thermophysical properties (conductivity k or conductivity tensor $\overline{\overline{k}}$ and total volumic heat denoted ρc here) may vary in space (heterogeneous case) and possibly with temperature (thermodependent properties of the material).

Knowledge of this heat flux allows calculating the rate of heat flow Φ (W) that goes through any surface of area A:

$$\Phi = \int_A \vec{\boldsymbol{q}} \,.\, \vec{\boldsymbol{n}} \; \mathrm{d}A \tag{3.3}$$

where $\vec{\boldsymbol{n}}$ is the local outward normal pointing (with respect to A) unit vector.

Thermal conductivity of materials can vary significantly with temperature.
Thermal diffusivity is defined as the ratio of the thermal conductivity and the specific heat per unit volume:

$$a = \frac{k}{\rho c} \tag{3.4}$$

2.2 Objective of a model

The model-builder has a given objective : he tries to represent the real physical system by a model ***M***, that will be used to simulate its behaviour. This model requires the knowledge of a given number of structural parameters, which form what is called a "parameter vector" $\boldsymbol{\beta}$. Its objective is to get identical responses of both system, $y(t)$, and model $y_{mo}(t; \boldsymbol{\beta}, u)$, under the excitation by an identical time-varying stimulus u (t), see figure 1 which corresponds to the case of example 1 further down.

If the control science terminology is used, this stimulus is called « input » and the response « output ». These two terms have no geometrical meaning here.

In heat transfer, the stimulus is produced either by a source, that is for example a surfacic thermal power (absorption of a radiative incident flux by a solid wall for example) or an internal power (Joule effect produced by an electrical current, heat of reaction of a chemical reaction,…). It can also be an imposed temperature difference (temperature difference between the inside and outside air environments on both sides of a solid wall for example).

Let us note that if steady state regime is considered, both stimulation u and measured y or model y_{mo} responses do not vary with time.

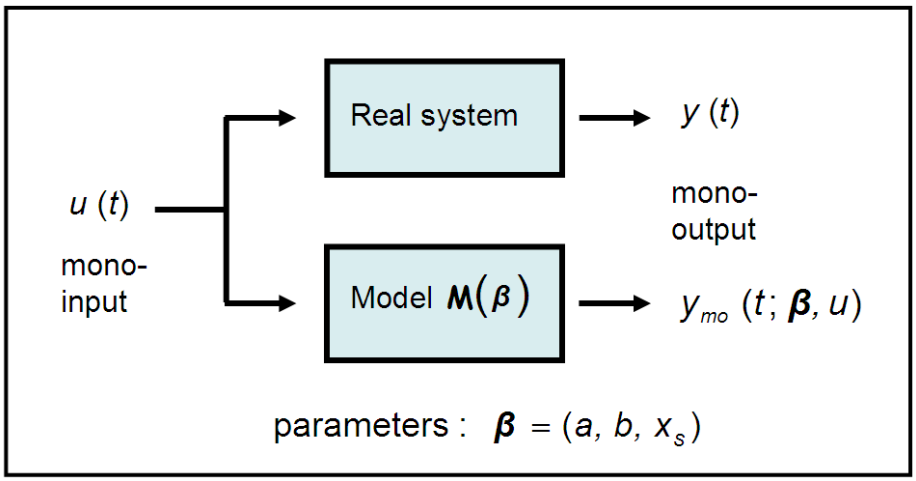

Figure 1. Real system and its representation by a model (case of a zero initial temperature field)

2.3 Internal and external representations, parameterizing, state model and model structure

2.3.1 Example 1 : mono input/mono output case

Figure 2 shows a semi-infinite medium in the x direction, whose front face (x = 0) is stimulated by a heat flux u (W m^{-2}) at initial time t = 0. The initial temperature distribution T_0 (x) may be non uniform. A temperature sensor is embedded at a dept x_s inside the medium and delivers a signal y. So, starting at initial time, a transient one-dimensional temperature field T (x, t) develops inside the medium.

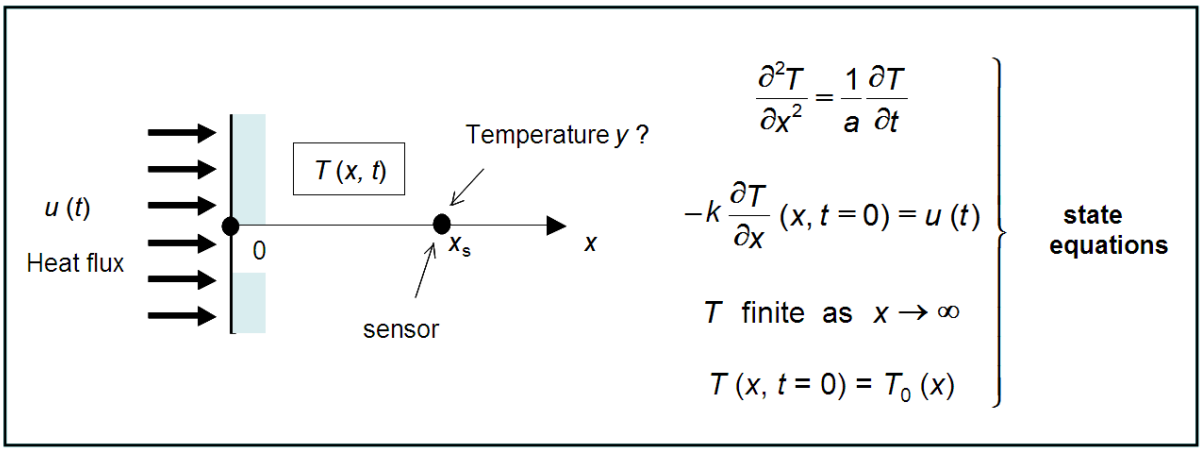

Figure 2. Response of a temperature sensor embedded inside a semi-infinite medium

This temperature field, also called « state » of the system, is the solution of the heat equation, a partial derivative equation here, as well as of its associated boundary and initial conditions.

These equations are called **state equations** of this thermal system.
Different structural parameters appear in these equations: the medium heat conductivity k ($W.m^{-1}.K^{-1}$), its thermal diffusivity $a = k/\rho c$ ($m^2.s^{-1}$), where ρ and c are its density ($kg.m^{-3}$) and its specific heat ($J.kg^{-1}.K^{-1}$). The theoretical signal of the sensor y_{mo} (response of the model), caused by the medium stimulation u, is given by the **output equation**.

$$y_{mo}(t) = T(x_s, t) \tag{3.5}$$

The state equations give an **internal representation** of the **direct problem** that allows the calculation of the system response everywhere, for a known excitation, while the sensor response is given by the output equation.

The state equations can be solved analytically here and calculation of the output can be directly implemented, because the system is *causal*, *linear* and invariant in time, see Ozisik [2]:

$$y_{mo}(t) = \int_0^{\infty} G(x_s, x, t)\, T_0(x)\, \mathrm{d}x = \int_0^{t} Z(t-\tau)\, T_0(x)\, u(\tau)\, \mathrm{d}\tau = y_{mo\ relax}(t) + y_{mo\ forced}(t) \tag{3.6}$$

with:

$$G(x_s, x, t) = \frac{1}{2\sqrt{\pi\, a\, t}} \left[\exp\left(-\frac{(x_s - x)^2}{4\, a\, t} \right) + \exp\left(-\frac{(x_s + x)^2}{4\, a\, t} \right) \right] \tag{3.7}$$

$$Z(t) = \frac{1}{b\sqrt{\pi\, t}} \exp\left(-x_s^2 / 4at \right) \tag{3.8}$$

where $G(x_s, x, t)$ is the Green's function associated to relaxation, at location x_s, of the initial temperature field $T_0(x)$ at location x, and $Z(t)$ the transfer function of the system**,** while $b = (k\rho c)^{1/2}$ is the thermal effusivity of the medium.

Equation (3.6) shows that two effects overlap: the first term corresponds to relaxation of the initial temperature field (free solution that vanishes for long times) while its second term, a convolution product, corresponds to the response ("forced" solution) to the heat flux excitation. Transfer function Z, that links a temperature response to an excitation power is called a time impedance, the same way as in AC electrical circuits. This function, once convoluted with the flux excitation u, yields the forced component of the temperature signal of the model. This can be expressed by a simple product of the corresponding Laplace transforms:

$$\bar{y}_{mo\ forced}(p) = \bar{Z}(p)\, \bar{u}(p) \qquad \text{with } \bar{f}(p) = \int_0^{\infty} f(t) \exp(-pt)\, \mathrm{d}t \tag{3.9}$$

If initial temperature T_0 is uniform in the medium, the first term in $y_{mo}(t)$ in equation (3.6) becomes equal to T_0. This last equation constitutes an *external representation* of the direct problem. It bypasses the need for calculating state $T(x, t)$ of the modelled system.

The (theoretical) output of the model depends on three parameters : the two thermophysical properties of the medium's material, *a* et *b*, and on a parameter that relates to the sensor, that is its location x_s. These three parameters can be gathered in a specific parameter vector $\boldsymbol{\beta} = [a \;\; b \;\; x_s]^T$. This parameter vector $\boldsymbol{\beta}$ contains the structural parameters of the problem: it does not change when input $u(t)$ and/or initial state $T_0(x)$ change, see figure 1.

- **Important point on notation**
  Let us precise the notation that will be adopted now on:

  - a scalar, or a scalar function depending continuously on an other scalar or vector variable (time *t* or temperature *T*, or parameter column vector $\boldsymbol{\beta}$ for example) will be noted in non-bold italic characters (*k*, or $T(t, x)$ for example),

  - a column vector ($\boldsymbol{\beta}$, or $\boldsymbol{u}$, or $\boldsymbol{U}$, see eq. (3.13) further down) or a column vector function will be noted in bold lower or upper case italic characters,

  - a matrix, or a matrix function will be noted in bold upper case italic characters (matrix $\boldsymbol{A}$ or matrix function $\boldsymbol{E}$, see equation (3.14) further down, except if this matrix function is a standard explicit function, such as the exponential of a matrix, noted **exp** (.) here.

The previous structural parameters $\boldsymbol{\beta}$, input u and initial state T_0 can be assembled in a unique **list** (not a column vector made of scalar quantities here) of explanatory quantities $x = \{\boldsymbol{\beta}, u(t), T_0(x)\}$ gathering all the data necessary for the calculation of output y_{mo}.

Result of this modelling is sketched in figure 3.

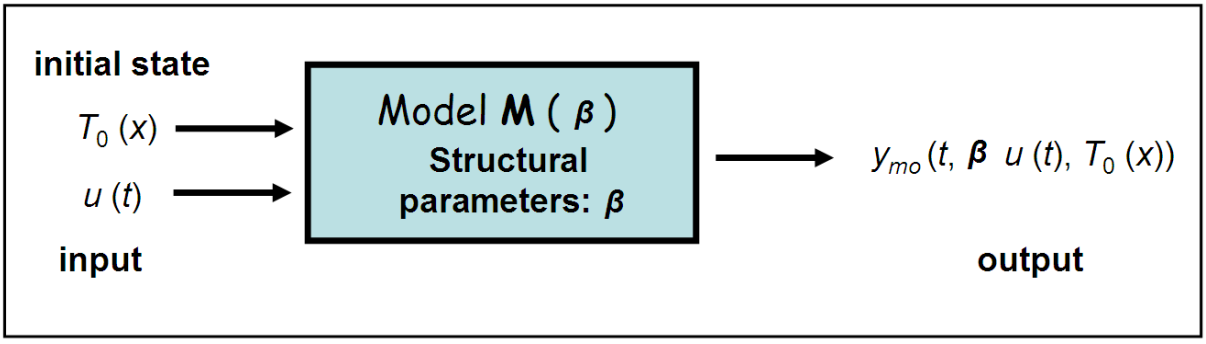

Figure 3. Input/output model for a thermal system

2.3.2 Parameterizing a function

In the previous list *x* of explanatory quantities, one can find scalar parameters (diffusivity, lengths, …) corresponding to structural parameters, as well as a time function $u(t)$, here a

heat flux. Other functions can appear such a non uniform initial state $T_0(\mathrm{P})$, or a non uniform structural parameter $\beta(\mathrm{P})$ or a parameter depending on temperature $\beta(T)$.

We suppose here that such a function is a time-depending input $x = u(t)$. In order to be able to deal with this kind of function, in the simulation (direct) problem and also in the inverse problem (finding *u* from measured *y*'s, where this aspect becomes of prime importance), this function has to be parameterized by its projection on a selected basis of *n* chosen functions $f_j(t)$:

$$u_{\text{param}}(t) = \sum_{j=1}^{n} u_j \; f_j(t) \tag{3.10}$$

The new function u_{param}, replaced now by a vector $\boldsymbol{u} = [u_1 \;\; u_2 \;\; \cdots \;\; u_n]^T$ of finite size *n*, is an approximation of the original *u* function, that can consequently be considered as a vector with an infinite number of components. This approximation, that we will call "**parameterization**" now on, generates an a priori error that depends both on the chosen basis and on its size.

Figure 4 shows two possible choices, using a constant time step $\Delta t = t_j - t_{j-1}$:

- in case a) the u_j components are the discrete values of the original function on the time grid and « hat » functions are selected as basis functions, see Figure 4a;
- in case b) these components are averaged values of this function over one time step and « door » functions are selected for this basis, see Figure 4b.

Choice for the basis is not unique and strongly depends on the problem at stake.
So hat function *parameterization* of case a) corresponds to linear interpolation using a table of discrete values; this parameterization choice is appropriate if a temperature dependency has to be modelled, for thermal conductivity $k(T)$ for example. In that case time *t* has to be replaced by temperature *T* in the basis functions that become $f_j(T)$.

In case b), a piecewise constant function basis has been chosen. It suits deconvolution inverse problems, such as a time-varying source estimation using an experimental temperature response.

In both cases, each u_j component requires, for its calculation, knowledge of function $u(t)$ within the neighbourhood of time t_j only. Use of such *local* bases is convenient because they directly derive from the time-space gridding. It is also possible to use projections on *non local* bases such as polynomials, exponentials, trigonometric functions…

The choice for a type of parameterization is very large. Constraints can be a priori set for the functions of the basis: they can present various properties such as monotony, regularity (continuous function with continuous first and second derivatives), positivity, or they can be assigned fixed values on part of their time domain $[t_{inf} \;\; t_{sup}]$. One can also think of B-splines bases , wavelets bases …

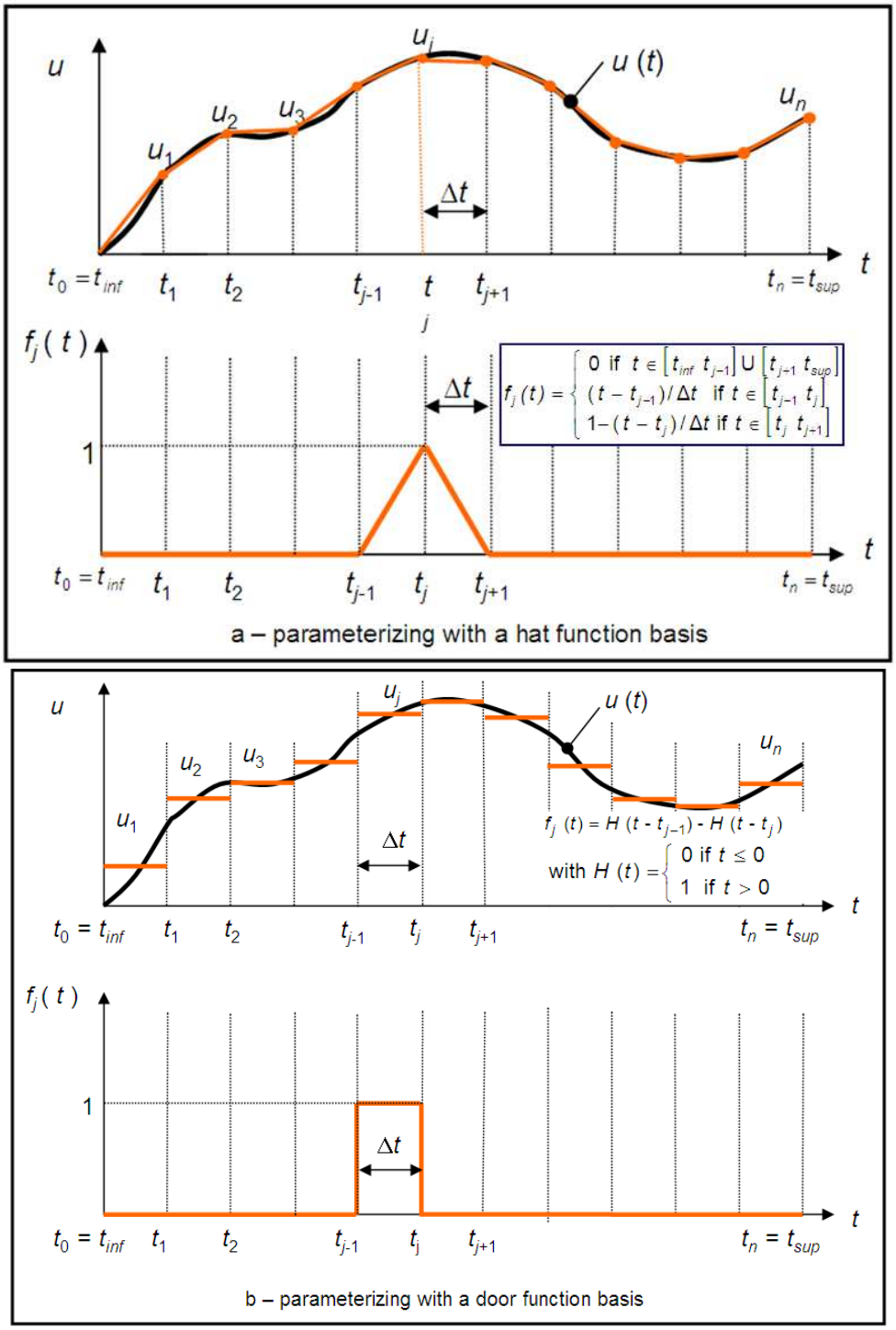

Figure 4. Parameterization of a function

Remark

Use of orthogonal function bases is possible. They correspond to functions $f_j(t)$ such as:

$$\int_{t_{inf}}^{t_{sup}} f_j(t)\, f_k(t)\, \mathrm{d}t = N_j\, \delta_{jk} \tag{3.11}$$

where δ_{jk} is Kronecker symbol ($\delta_{jk} = 0$ if $k \neq j$ and $\delta_{jk} = 1$ otherwise) and N_j the square of the norm of function f_j.

Door functions shown in Figure 4b are orthogonal, but it is not the case for hat functions shown in 4a.

It is very interesting to choose the eigenfunctions of the heat equation (they can be found using the method of separation of variables [2]) for these $f_j(t)$ functions. In that case, the components of the corresponding ***u*** vector become integral transforms, that is the different harmonics, of the original function [3]. This method is related to Singular Value Decomposition [4].

2.3.3 State-space representation for the heat equation

The one-temperature heat equation can be written, for a thermal diffusion problem in an anisotropic medium as the following partial differential equation:

$$\begin{aligned} &\mathrm{div}\left(\overline{\overline{k}}\ \mathbf{grad}\,(T)\right) + q_{vol} = \rho c \frac{\partial T}{\partial t} \\ &+ \ \text{boundary, interface and initial conditions} \end{aligned} \tag{3.12}$$

Here q_{vol} designates the volumic heat sources (W.m^{-3}) but other sources, such as surface sources, may be present in the boundary or interface conditions. $\overline{\overline{k}}$ designates the conductivity tensor here. This partial differential equation system is of the evolution type and can be considered as a dynamical system. So, its solution, the temperature field $T(t, \mathrm{P})$, that is continuous in time, constitutes the state of the system, that can be noted here $T_{\mathrm{P}}(t)$, that is, for a given time *t*, a vector in an infinite dimension space.

This system that corresponds to a *distributed parameter system* can be discretized in space, using *N* nodes, the discretized state becoming a vector $\boldsymbol{T}(t)$ in a *N* dimension space. The resulting state equation of this system takes the form of a *lumped parameter system* that corresponds to a system of first ordinary differential equations:

$$\frac{\mathrm{d}\boldsymbol{T}}{\mathrm{d}t} = \boldsymbol{E}\,(\boldsymbol{T}, \boldsymbol{U}, t) \qquad \text{with} \quad \boldsymbol{T}\,(t = t_0) = \boldsymbol{T}_0 \tag{3.13}$$

where vector $\boldsymbol{U}(t) = \left[u_1(t) \quad u_2(t) \quad \cdots \quad u_p(t)\right]^T$ corresponds to a local parameterization in space, but not in time, of the volumetric distributed source $q_{\mathrm{vol}}(\mathrm{P}, t)$ and of the other sources possibly present in the boundary or interface conditions. The number of different parameterized sources is called *p* here.

Let us note that this equation is written here in the very general case of a fully non linear system where temperature is the only state variable: conductivity or volumetric heat may depend on temperature or the associated interface/boundary conditions may not be linear (radiative surface heat losses for example). In that case, matrix $\boldsymbol{E}$ depends on temperature $\boldsymbol{T}(t)$ in a non linear way while matrix $\boldsymbol{B}$ may possibly depend on temperature. In a similar way, stimulation vector $\boldsymbol{U}$ may also be temperature dependent. In that case, each of the p components u_j of $\boldsymbol{U}$ is an implicit function of time, since it depends on the present and past states of the system, that is on $\boldsymbol{T}$ on the [0 t_0] interval.

We assume to be in the linear case (linear heat equation system and linear source) here on:

$$\boldsymbol{E}\ (t, \boldsymbol{T}, \boldsymbol{U}) = \boldsymbol{A}\ \boldsymbol{T} + \boldsymbol{B}\ \boldsymbol{U} \quad \text{with} \quad \boldsymbol{A} \text{ and } \boldsymbol{B}\text{: constant matrices} \tag{3.14}$$

The different vectors and matrices present in the linear form of the state equation (3.13-3.14) are thus defined in figure 5.

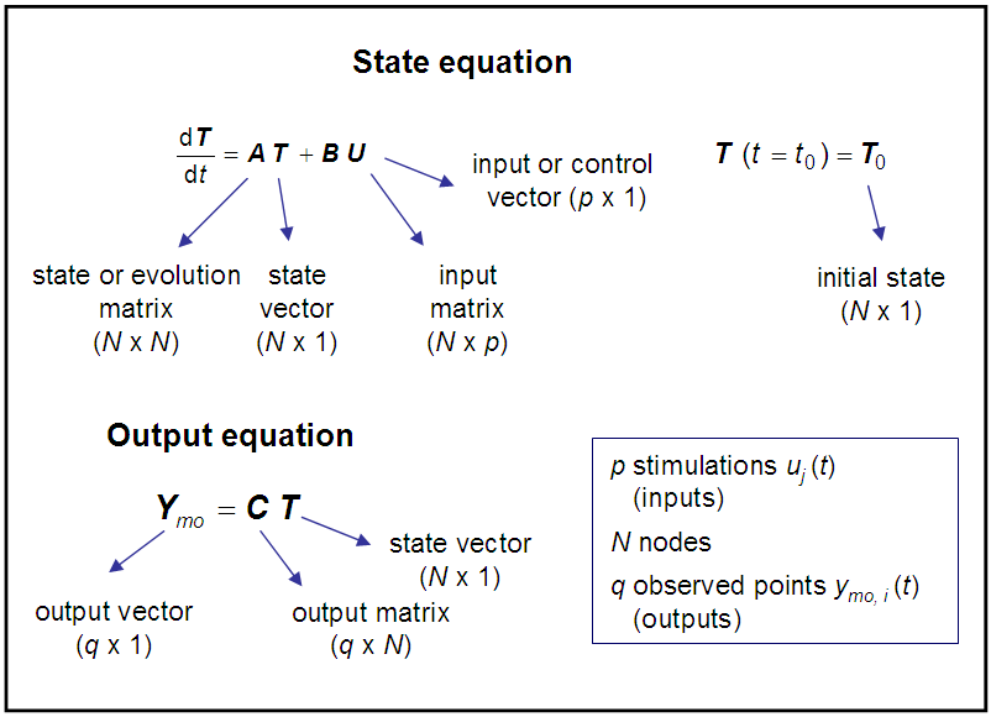

Figure 5. State and output equations of a linear dynamical thermal system

An analytical solution for the state vector $\boldsymbol{T}(t)$ of this *state-space representation* of a linear system, can be found formally using the exponential function of a matrix :

$$\boldsymbol{T}\ (t) = \mathbf{exp}\ (\boldsymbol{A}\ (t - t_0))\ \boldsymbol{T}_0 + \int_{t_0}^{t} \mathbf{exp}\ (\boldsymbol{A}\ (t - \tau))\ \boldsymbol{B}\ \boldsymbol{U}\ (\tau)\ \mathrm{d}\tau \tag{3.15}$$

In practice, and in the case of implementation of an inverse technique, all the N components of the state vector (temperatures at the different nodes of the model here) do not present the

same interest: only a subset, that is a number q ($q \leq N$) of its components are selected as model outputs. They can correspond to observations provided by q sensors for example. These outputs are numbered and called $y_{mo,i}$ and they are put in an *output vector* $\boldsymbol{y}_{mo}$:

$$\boldsymbol{Y}_{mo}(t) = \left[y_{mo,1}(t) \quad ... \quad y_{mo,i}(t) \quad \cdots \quad y_{mo,q}(t) \right]^T \tag{3.16}$$

Output vector $\boldsymbol{y}_{mo}$ is linked to state vector $\boldsymbol{T}$ through an output matrix (or observation matrix) $\boldsymbol{C}$, of q x N dimensions: the coefficients of this observation matrix are either 0's or 1's, according to the observed nodes:

$$\boldsymbol{Y}_{mo}(t) = \boldsymbol{C}\,\boldsymbol{T}(t) \tag{3.17}$$

This equation is also called the *output equation*.

The response of the system, that is the observed output, can be calculated thanks to equations (3.17) and (3.15) as:

$$\boldsymbol{Y}_{mo}(t) = \boldsymbol{C}\ \mathbf{exp}\left(\boldsymbol{A}\,(t - t_0)\right)\boldsymbol{T}_0 + \boldsymbol{C}\int_{t_0}^{t} \mathbf{exp}\left(\boldsymbol{A}\,(t-\tau)\right)\boldsymbol{B}\,\boldsymbol{U}(\tau)\,\mathrm{d}\tau \tag{3.18}$$

One notices, in a very similar way as in the previous example (3.6), that this response is the sum of a term corresponding to the relaxation of initial state $\boldsymbol{T}_0$, that is the free regime, and a convolution product term corresponding to response to stimulation $\boldsymbol{U}(t)$, the forced regime.
The meaning of the notion of state appears clearly here: knowledge of the state of the system at a given time $\boldsymbol{T}(t_0)$ as well as the history of the different sources for the $]t_0\ t]$ time interval allows calculating the current state $\boldsymbol{T}(t)$ of the material system. So, at a given time, the thermal state contains the whole past of the system.

Remark 1

Equation (3.12) can easily be generalized to the case of heat transport in a pure fluid:

$$\begin{aligned} &\mathrm{div}\,(\overline{\overline{k}}\ \mathbf{grad}\,T) - \rho c_f\ \boldsymbol{v}\ .\ \mathbf{grad}\,T + q_{vol} = \rho c\ \frac{\partial T}{\partial t} \\ &+ \text{ boundary, interface and initial conditions} \end{aligned} \tag{3.19}$$

In this equation, an additional term appears with respect to the pure diffusion case (3.12), the advection term. It is based on the volumetric heat of the fluid $\rho c_f = \rho c$ and on the fluid velocity $\boldsymbol{v}$ (solution of the Navier-Stokes and continuity equations) and on a conductivity tensor $\overline{\overline{k}}$ that reduces simply to the thermal conductivity k of the fluid.

In the case of heat dispersion in a porous medium, this velocity has to be replaced by a local Darcy velocity, temperature T becomes an average "enthalpic" temperature at the local scale (for the one-temperature model), while $\overline{\overline{k}}$ becomes the thermal dispersion tensor,

whose coefficients depend on this local Darcy velocity. In this case, ρc , the volumetric heat in the transient storage term, differs from ρc_f . This total volumetric heat ρc results from a mixing law and represents the total volumetric heat of both fluid and solid phases, using the local volume fractions as weights [5].

Remark 2

State of a thermal system is not always composed of the sole temperature *T*. Two different examples of a composite state are given next.

If a physical or chemical transformation occurs inside the modelled material, a polymerisation of a thermoset resin for example, a heat source appears because of the heat of reaction. It usually depends on the degree of advancement of the reaction, through a kinetic law. This degree of advancement constitutes the second state variable. In that case, the state equations are composed of the heat diffusion equation (3.12) completed with a coupled mass balance equation for each of the species present in the reacting system.

Another example can be given for coupled conduction and radiation heat transfer in semi-transparent media. The radiative intensity is the second state variable and the radiative transfer equation (an integro-differential of equation) will be associated with the heat diffusion equation in order to constitute the new state equations.

Remark 3

When a steady state $\boldsymbol{T}_{ss}$ corresponding to an input vector $\boldsymbol{U}_{ss}$ exists, equations (3.13) allows its calculation: it is written with d$\boldsymbol{T}$/dt = 0, which yields in the fully linear case, see equations (3.13) and (3.14):

$$\boldsymbol{T}_{ss} = -\boldsymbol{A}^{-1}\,\boldsymbol{B}\,\boldsymbol{U}_{ss} \quad \Rightarrow \quad \boldsymbol{y}_{mo,ss} = -\boldsymbol{C}\,\boldsymbol{A}^{-1}\,\boldsymbol{B}\,\boldsymbol{U}_{ss} \tag{3.20}$$

2.3.4 Model terminology and structure

All the equations and necessary conditions for calculating the output of the model constitutes the structure of the model, which can be written as a functional relationship, for a single output variable:

$$y_{mo} = \eta\,(t, x) \quad \text{or} \quad y_{mo} = \eta\,(t, \boldsymbol{x}) \tag{3.21a, b}$$

where x is either a *list* of explanatory quantities, including functions, $x = \{\boldsymbol{\beta}\ ,\ u\ (\mathrm{P}, t), T_0(\mathrm{P})\}$ (3.21a) or its vector version $\boldsymbol{x} = [\,\boldsymbol{\beta}\quad \boldsymbol{U}\quad \boldsymbol{T}_0\,]^T$ (3.21b) , built with functions *parameterized* in space, *and* time (or in temperature, for non linear problem with thermal dependency of either input u or structural parameters β_j's).

When several output variables can be observed, one deals with an output vector (not a scalar y_{mo} anymore) which requires the use of a vector function $\boldsymbol{\eta}(.)$ whose arguments are time t and either the x list or its vector version $\boldsymbol{x}$:

$$\boldsymbol{y}_{mo} = \boldsymbol{\eta}\,(t, x) \quad \text{or} \quad \boldsymbol{y}_{mo} = \boldsymbol{\eta}\,(t, \boldsymbol{x}) \tag{3.22 (a, b)}$$

A wider meaning can be given for vector $\boldsymbol{U}$ in this last definition of parameter vector $\boldsymbol{x}$: this vector can represent, in a non linear case, a temperature dependent stimulus u (T) that has been parameterized. Let us note that a temperature dependent thermophysical property $\beta_j(T)$, once parameterized, gives rise to constant coefficients for parameter vector $\boldsymbol{\beta}$. Coefficients of vector $\boldsymbol{\beta}$ can also stem from a space dependent property $\beta_j(\mathrm{P})$, that has been parameterized, in the case of a heterogenous medium.

The "*direct problem*" consists in finding model output $y_{mo}(t; x)$ at a given time t in the $[t_0\ t_{final}]$ interval, for known data $x = \{\boldsymbol{\beta}, u(\mathrm{P}, t), T_0(\mathrm{P})\}$. Solution of this problem can allow further numerical simulations of the output behaviour.

A model relies on a given *structure*, that is a functional relationship, noted η above, between the output variable (or explained or dependent variable) y_{mo} (an observed temperature here) and the independent variable (time t for transient problems) and a parameter vector $\boldsymbol{x}$, whose components are the parameterized explanatory quantities. It is important to remind that aside the previous structure, parameters $\boldsymbol{x}$ of the model should be defined accordingly, see figure **6**. They can either have a physical meaning if a state modelling is performed, or simply a mathematical meaning without clear physical interpretation if an identified modellization is implemented.

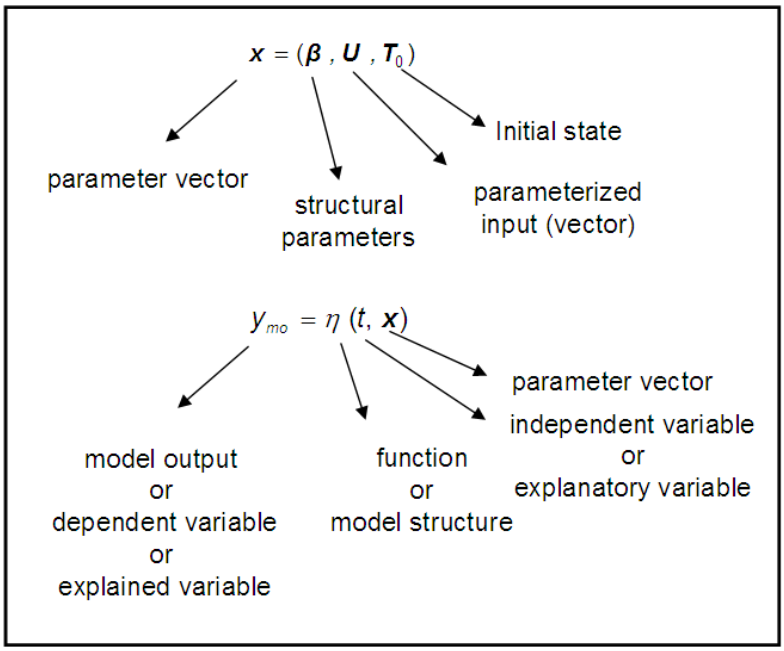

Figure 6. Parameter vector and structure of a model

One can notice that a model, in case of a single output, can provide not only a scalar output y_{mo} depending continuously on time t, but also a vector output $\boldsymbol{y}_{mo}$. This output column vector is associated with the same output variable, a local temperature for example, sampled at different times $t_1, t_2, \cdots, t_m$, or can result from a sampling of the explanatory

variable, that can be a space coordinate for a steady state problem. It can also gather in a single column vector, of length *qm*, several output temperatures observed at different points P_i (i = 1 to q), sampled for m different times t_k.

2.4 Direct and inverse problems

2.4.1 Direct problem

We have seen above, when the studied problem allows it, that the usual approach of the thermal science scientist consists in constructing a *knowledge-based model*, such as equations (3.18), in order to be able to simulate the behaviour of the physical system.

This leads to a numerical or analytical solution of a partial differential equation in the case of a heat diffusion problem (or an integro-differential system of equations for radiation heat transfer in semi-transparent media, temperature and radiative intensity being the state variables) that represent the corresponding transfer of heat. Solution of these equations also requires the knowledge of the conditions at the boundaries (Dirichlet, Neumann, Fourier,…) or at the internal interfaces (for a medium composed of different materials) as well as the initial condition in the system.

If an internal representation is adopted (*white box model*), several quantities of different nature have to be introduced in the state (3.13) and output equations $y_{mo}(t) = T(t, P_i)$ of the model, written for a single temperature sensor located at point P_i. If the output is observed at q such points for m times set into a time vector $\boldsymbol{t} = [t_1 \; t_2 \cdots \; t_m]^T$ it becomes an output vector $\boldsymbol{y}_{mo}(\boldsymbol{t}; \boldsymbol{x})$ that depends also on parameter vector $\boldsymbol{x}$, where this vector is composed of :

- the raw u (P, t) or parameterized $\boldsymbol{U}(t)$ excitation;
- vector $\boldsymbol{\beta}_{struct}$ of structural parameters, a and b in example 1 or coefficients of matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ in the linear state equations (3.13)-(3.14);
- vector $\boldsymbol{\beta}_{pos}$ describing the position of the observation, x_s in example 1 and coefficients of matrix $\boldsymbol{C}$ in output equation(3.17);
- the initial temperature field T_0 (P) or its parameterized version $\boldsymbol{T}_0$.

Input variables u (P, t) are controlled by the user: they are either power sources or imposed temperature differences, inside or outside the system, that make temperature and output depart from a zero value in case of zero initial temperature T_0 (P).

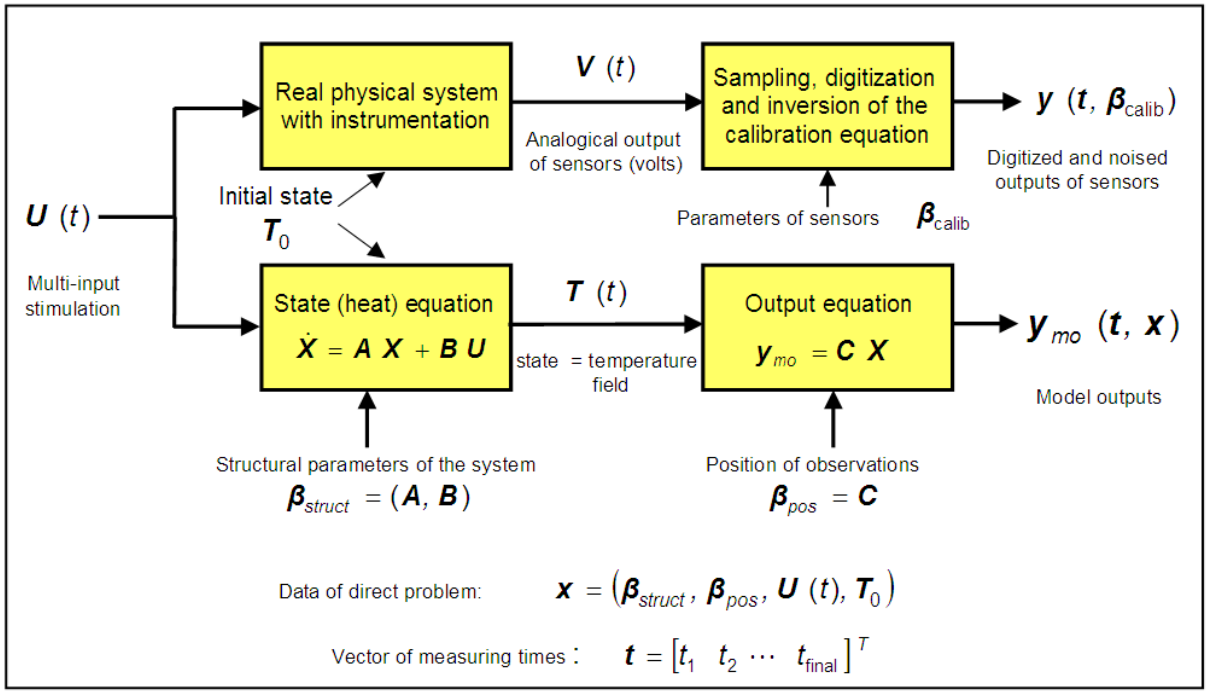

Figure 7. Linear model and material system with temperature measurement.

Structural parameters $\boldsymbol{\beta}_{struct}$ characterize the system. They can be :

- geometrical quantities (shape and dimensions of the system),
- thermophysical properties : conductivities , volumetric heats, heat transfer coefficients, emissivities, contact or interface resistances,…

The relationship between output variables, generally a subset of the state, and state variables, the temperature field, makes the previous position parameter vector $\boldsymbol{\beta}_{pos}$ appear in this output equation.

A functional scheme corresponding to linear state and output heat equations is shown in the lower line of figure 7.

This corresponds to the usual process of a model-user: for a known initial state $\boldsymbol{T}(t_0)$, a known excitation $\boldsymbol{U}$ (t) and known structural parameters, the heat equation and the output equations are solved sequentially to calculate the theoretical response $\boldsymbol{y}_{mo}$ of the sensors. This output corresponds to possible temperature measurements at the same locations (upper line in figure 7). The **direct problem** can thus be solved.

2.4.2 Inverse problem approach

The preceding analysis shows that any variation in the data represented inside the $\boldsymbol{x}$ vector (including structural and position parameters $\boldsymbol{\beta}_{struct}$ and $\boldsymbol{\beta}_{pos}$) will produce a variation of the $\boldsymbol{y}_{mo}$ output.

Conversely, any variation of this output $\boldsymbol{y}_{mo}$ is necessarly caused by variation of some data inside $\boldsymbol{x}$.
The inverse approach is based on this principle. When knowledge of part of the variables that are necessary to solve the direct problem is lacking, data vector $\boldsymbol{x}$ of this problem can be split into two vectors the following way :

$$\boldsymbol{x} = \begin{bmatrix} \boldsymbol{x}_r \\ \boldsymbol{x}_c \end{bmatrix} \tag{3.23}$$

where $\boldsymbol{x}_r$ now represents the (column) vector gathering the unknown part of the data that are *sought* (*researched*), and $\boldsymbol{x}_c$ its *complementary* part that contains *known* data.

In that case, solving the direct problem constitutes an impossible task. Any process aimed at finding $\boldsymbol{x}_r$ requires some *additional information.*

Problems whose objective is to find a value for $\boldsymbol{x}$, starting from additional information(s), are called *inverse problems*.

Any inverse problem consists in making the model work in the « backwards » way : if outputs $\boldsymbol{y}$ as well as model structure η are known, part $\boldsymbol{x}_r$ of $\boldsymbol{x}$ will be sought, its complementary part being known, see figure 8.

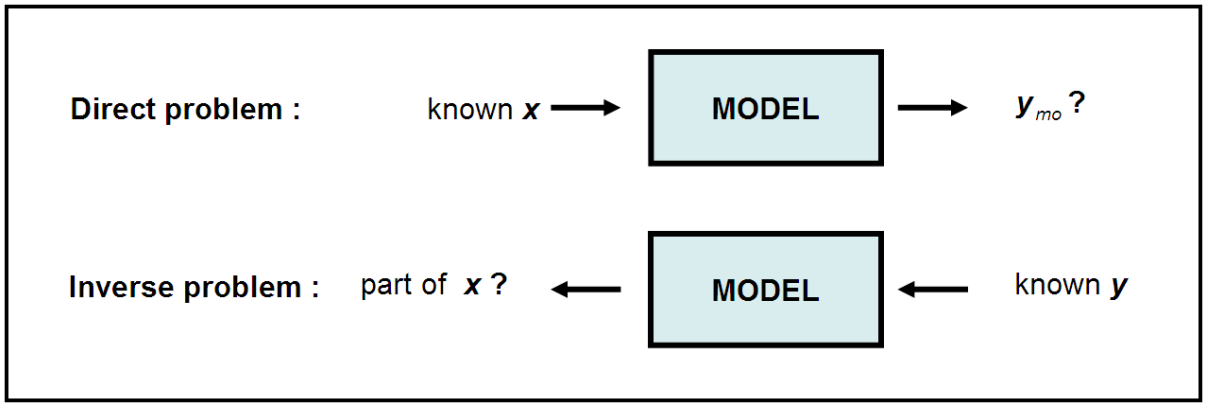

Figure 8. Direct problem/Inverse problem

2.4.2 Inverse problems in heat transfer, case of inverse measurements problems

2.4.2.1 Different types of inverse problems in heat transfer

The nature of the previous *additional information* necessary for solving any inverse problem allows to bring out three main types of problems :

- *inverse measurement problems*, where this information stems from output signal $\boldsymbol{y}$ of sensors;

- *control problems*, where the previous measurements are replaced by desired values of either the state $T(\mathrm{P}, t)$ or output variables $\boldsymbol{y}$: data or $\boldsymbol{y}$ are the targets. In this class of problem, the sought quantity is generally the stimulus $u(\mathrm{P}, t)$, ort the initial state $T_0(\mathrm{P})$, but it can also be a structural parameter (a velocity or a flow rate in a forced convection cooling problem for example). In this class of problems, it is not always possible to reach the targets, for physical or mathematical reasons, and it may be necessary to specify a certain number of constraints on the sought solution.

- *system identification problems,* that is model construction for simulating the behaviour of a system, see lecture 8 in this school. These can be classified into two categories:

i) *model reduction* : $\boldsymbol{y}$ is the output of a *detailed* model $\eta_{\mathrm{det}}\ (t\ ;\ \boldsymbol{x}_{\mathrm{det}})$ completely known and the structural parameters (part of $\boldsymbol{x}_{\mathrm{red}}$) of a *reduced* model $\eta_{\mathrm{red}}\ (t\ ;\ \boldsymbol{x}_{\mathrm{red}})$ of given structure η_{red} are sought, both models sharing either identical or close stimulations $u(\mathrm{P}, t)$ and initial state $T_0(\mathrm{P})$, that are parts of $\boldsymbol{x}_{\mathrm{det}}$ and $\boldsymbol{x}_{\mathrm{red}}$. This can be written:

$$\eta_{\mathrm{det}}\ (t\ ;\ \boldsymbol{x}_{\mathrm{det}}) \approx \eta_{\mathrm{red}}\ (t\ ;\ \boldsymbol{x}_{\mathrm{red}}) \tag{3.24}$$

where $\boldsymbol{x}_{\mathrm{det}} = \left[\, \boldsymbol{\beta}_{\mathrm{det}} \quad \boldsymbol{U}_{\mathrm{det}} \quad \boldsymbol{T}_{0\ det} \,\right]^T$ and $\boldsymbol{x}_{\mathrm{red}} = \left[\, \boldsymbol{\beta}_{\mathrm{red}} \quad \boldsymbol{U}_{\mathrm{red}} \quad \boldsymbol{T}_{0\ red} \,\right]^T$

with, for mathematical reduction :

$$\begin{aligned} u_{\mathrm{red}}(\mathrm{P}, t) = u_{\mathrm{det}}(\mathrm{P}, t) \quad &\Rightarrow \quad \boldsymbol{U}_{\mathrm{red}} = \boldsymbol{U}_{\mathrm{det}} \\ T_{0\ \mathrm{red}}(\mathrm{P}, t) = T_{0\ \mathrm{det}}(\mathrm{P}, t) \quad &\Rightarrow \quad \boldsymbol{T}_{0\ det} = \boldsymbol{T}_{0\mathrm{red}} \end{aligned} \tag{3.25}$$

or, for physical reduction:

$$\begin{aligned} u_{\mathrm{red}}(\mathrm{P}, t) \approx u_{\mathrm{det}}(\mathrm{P}, t) \quad &\Rightarrow \quad \boldsymbol{U}_{\mathrm{red}} = f_U\ (\boldsymbol{U}_{\mathrm{det}}) \\ T_{0\ \mathrm{red}}(\mathrm{P}, t) \approx T_{0\ \mathrm{det}}(\mathrm{P}, t) \quad &\Rightarrow \quad \boldsymbol{T}_{0\ \mathrm{red}} = f_{T0}\ (\boldsymbol{T}_{0\ \mathrm{det}}) \end{aligned} \tag{3.26}$$

In both cases, *mathematical* or *physical model reduction*, the structural parameters of the reduced model depend on the corresponding parameters of the detailed model:

$$\boldsymbol{\beta}_{\mathrm{red}} = f_\alpha\ (\boldsymbol{\beta}_{\mathrm{det}}) \qquad \text{for} \qquad \alpha = u \ \text{ or } \ T_0 \tag{3.27}$$

but this relationship, function f_α, is explicit for physical reduction (see section 3.2 below), while it is not generally the case for mathematical reduction.

ii) *experimental model identification*: $\boldsymbol{y}$, $\boldsymbol{U}$ and $\boldsymbol{T}_0$ are measured, or supposed to be known, and the structural parameters (part of $\boldsymbol{x}$) of a model $\eta\ (t\ ;\ \boldsymbol{x})$ of given structure η, are known, $\boldsymbol{U}$ and $\boldsymbol{T}_0$ being their complementary part in $\boldsymbol{x}$.

Let us note that heat transfer modelling leads to models that can be either of the *white box* type, which means models based on first principles, eg. a model for a physical process from the Newton's equations, or of the *grey box* type (estimation of a transmittance function, by deconvolution from measured input and output, see lecture 8 in this advanced school), or even to models of the *black box* type, without any type of physical a priori on the model structure.

The previous state-state model (3.18), based on a heat balance and on Fourier's law defining heat flux, is of the *white box* type. The nature of the parameters in this class of models is perfectly known, which explains why they are used for thermophysical property estimation.

- Conversely, an identified model on an experimental basis, without a priori information on its structure, is also called a *black box* model: parameters of such a model have only a mathematical, but not physical, meaning. Such blax box models may for example derive from neural network modelling. In between, one can find *grey box* or *semi-physical* models: the model, that is the structure/parameters couple is chosen according to a certain physical insight on what is happening inside the system, and these parameters are estimated on an experimental basis.

2.4.2.2 Inverse measurement problems in heat transfer

We will focus here on *inverse measurement problems* where model structure (the equations) η is known and where measurements $y(t)$ are available on the time interval $[t_0\ t_{final}]$.
According to the nature of the explanatory variables $\boldsymbol{x}_r$ that are sought, solution finding for inverse problems may differ. One can distinguish in particular:

a) Inverse problems of *structural parameters estimation*: $\boldsymbol{x}_r \equiv \boldsymbol{\beta}_r$

System identification problems, of the black or grey box type, belong to this chategory: structural parameters (part of $\boldsymbol{x}$) of a ad'hoc $\eta(t; \boldsymbol{x})$ model are sought through experimental characterization. *Thermophysical property estimation* belongs to the white box category: *intrinsic* parameters, that is parameters that can be used for completely different simulation/experimental configurations, are sought through experimental characterization. In both types of problems, several experiments on the same setup, for the same sample, can be repeated in order to estimate the same unknown parameter(s).

b) Inverse *input* problems : $x_r \equiv u(\mathrm{P}, t)$

In heat transfer, this type of problem consists in finding the locations and values of the sources. Such a source, or excitation, is either a volumetric, surface, line or point heat source or simply a temperature difference imposed inside or at the boundaries of the system. It differs from the previous problem because the solutions sought are specific to each experiment made.

c) Inverse *initial state* problem : $x_r \equiv T_0(\mathrm{P})$

This problem is very close to the inverse input problem, since each fought solution is relative to a single given experiment.

d) Inverse *shape reconstruction* problems

In the previous types of inverse problems, boundaries of the domain are usually fixed and known. In certain cases (problems with change of phase, in welding or in solidification

applications, for example) shape of the domain (its boundary), or location of an interface between sub-domains (a change of phase moving front for example) has to be taken into account in the variables defining the direct problem. In the corrresponding inverse problem, the shape of this boundary has to be be first parameterized in order to be reconstructed through inversion.

e) Inverse problems of *optimal design/control*
A usual process aimed at reducing estimation errors, in a characterization process of type a), consists in coupling it to an optimal conception/control problem for the characterization experiment.
This optimization allows the design and the sizing of the experimental setup as well as the procedure for the experiments that will bring additionnal information necessary for this characterization.
This approach can provide a methodolodogy for a pertinent choice of inputs, locations of measurement points, and time observation windows, etc…Choice of these design quantities can be made in order to maximize a criterion based on the sensitivity of the output observations to the parameters that are sought.

Heat transfer characterization problems (that are structural parameters estimation or system identification problems) are usually non linear, which means that optimization of any design has to be implemented on the prior assumption that the sought parameters are known, with an iterative approach once a first estimation has been found. This means that *nominal* values of these parameters are necessary for such a design.

Remark

Use of any sensor, that very often delivers an electrical output quantity (a tension V, for example) requires the construction of a relationship between the quantity one wants to measure, temperature T here, and this instrument output.

It is therefore necessary to find, on the basis of the physical principle the sensor and the whole instrumental chain rely on, a model structure $V_{mo}(T\,;\,\boldsymbol{\beta}_{\text{calib}})$ where temperature is now the explanatory variable and where vector $\boldsymbol{\beta}_{\text{calib}}$ gathers all the parameters required for calculating the theoretical output temperature signal (thermoelectric power and cold junction temperature, in the case of a thermocouple sensor). Construction of the V_{mo} model and estimating parameters present in $\boldsymbol{\beta}_{\text{calib}}$ starting from simultaneous measurements of both V and T (using a reference temperature sensor) constitutes a *calibration problem*, that is, by nature, a parameter estimation problem, that is a type a) inverse problem (see section above) that has to be dealt with this way.

2.4.2.3 Measurement and noise, biased models

In *inverse measurements problems*, the additional information is brought by the measured output $y(t)$, that differs from the exact output $y^{exact}(t)$.

The difference $\varepsilon(t)$ between a sensor measurement y and the output of an ideal sensor $y^{exact}(t)$ giving the true temperature at the sensor location can be introduced :

$$y(t) = y^{exact}(t) + \varepsilon(t) \tag{3.28}$$

The sensor giving $y^{exact}(t)$ is ideal for two reasons:

i) its presence does not affect the local temperature of the medium (*non-intrusive* detector) and

ii) it provides the *true value* of its *own* temperature.

Equation (3.28) defines the measurement noise $\varepsilon(t)$, that can be considered as a random variable caused by the imperfect character of both instrumentation and of digitization of the signal. This noise is present, but its deterministic value can not be reached in practice.
This equation also shows that the measured signal is a random variable whose variance is the same as noise ε.

The assumption of a pertinent, that is non biased, model is made in practice:

$$y^{exact}(t) = y_{mo}\ (t,\ \boldsymbol{x}^{exact}) \tag{3.29}$$

where $\boldsymbol{x}^{exact}$ is the true value of the explanatory variables.

Verifying this assumption of consistency between model and measurements is crucial. Corresponding tools exist (study of the residuals, see lecture 4 in this advanced schoiol).

Remark
Equation (3.28) should be defined for discrete values $y_i = y(t_i)$, $\varepsilon_i = \varepsilon(t_i)$ and $y_i^{exact} = y^{exact}(t_i)$ corresponding to the sampling times t_i of the measured signal, of the exact temperature and of the noise respectively.

3. Choice of a model for the inversion

3.1 Challenges: objectives, structure, consistency, complexity and parcimony

Before constructing a model, the model-builder has to be clear about the way his model will be used, that is about the objective of such a modelling. The objectives depend of the application and can belong to one of the following categories that can be listed in a non limitative way:

- estimation of thermophysical properties
- heat source/flux estimation
- initial temperature field estimation
- defect detection and non destructive testing
- simulation of the system behaviour for better design or future state forecasting
- model reduction for faster computation or use for heat source/flux estimation

- conception of a model for closed-loop (feedback) control
- …

So the type of model will not be the same for each application, because the required model precision will differ: defect detection in a composite slab using infrared thermography [6] does not require a model with the same temperature resolution as in thermophysical property estimation, such as the flash method for liquid diffusivity estimation [7].

The accuracy of a model is determined by its consistency with the modelled physical situation, that is its ability to simulate closely the behaviour of the studied system. *Internal representation*, with the use of state-space models, should be generally favoured , because it provides a mathematical structure linked to the physics of the modelled problem « for free ». In addition, this type of representation allows to highlight the intrinsic parmeters of the system, that is its thermophysical properties or thermal resistances and impedances.

The purpose of the model that is used for inverting measurements is not to reproduce or to mimic the whole temperature field : it should only provide an output that can be compared to the sensor output signal at the *location* where this one is embedded. Structure, that is scalar or vector function η used above, is what defines a model. Its complexity should be adapted to the uncertainties associated with any description of a physical system: use of a model that is too much simplified (simple structure with a low number of structural parameters, such as a *lumped parameter* model, see next section) can introduce a systematic error, a bias, in its output variables, that could depart too much from model predictions and from the experimental observations to be used the inverse way. Conversely, choice of a too *detailed* model, with a high number of parameters:

- tends to make implementation of the inversion algorithm involved, or to make it numerically impossible or very difficult;
- may lead to unstable solutions for the inverse problem, because of noise amplification (in case of inversion of measurements) : the inverse problem becomes ill-posed.

A demonstration of this effect can be obtained through a Singular Value Decomposition of the scaled sensitivity matrix, in a non linear parameter estimation case: it is given by a calculation of the quadratic mean square of the relative standard deviation of the estimated parameters, in lecture 4 of this school (equation 55).

This dilemma pleads in favour of the use of *parcimonious* models for inverse use, that is models that provide a good balance between antagonist criteria of use of a minimum number of parameters on the one hand, and maximum agreement with reality (fidelity to measurements) on the other hand.

Up-to-date capacities of numerical simulation tools as well as structure of the *optimization* and *regularization* algorithms, allow to solve inverse problems with more and more complex models, using *mathematical model reduction* techniques. These allow a very significant reduction of the size of the state vector (temperature at different nodes of the numerical grid here. So reduction of a model, followed by its implementation in an inverse procedure, can bring an efficient approach for the most difficult cases, such as 3D heat transfer with change of phase or advecto-diffusive transfers within flowing fluids for example [8]. We will focus next on a different type of reduction technique, *physical model reduction*.

3.2 Example 2: Physical model reduction

In order to show that a thermal model can be reduced on a physical basis and that many models, of different complexity and resolution are available to simulate the same heat transfer situation (non-uniqueness of a model), we will consider heat transfer in a slab, whose characteristics are defined below:

- homogeneous rectangular slab, thickness *e*, lengths ℓ_x and ℓ_y in its plane
- thermal diffusivity and conductivity *a* and *k,* volumetric heat $\rho c = k / a$

This slab is stimulated by a surface power (absorption of solar radiation, for example) on its front face and temperature is measured at *q* points by sensors either embedded in the material or located on the front or rear face of the slab, see figure 9. The slab is supposed to be insulated on its four (lateral) sides, and exchanges heat with the surrounding environment T_∞ only on its rear face through a uniform heat transfer coefficient *h* that represent its losses (convection and linearized radiative losses). Its initial temperature T_0, at time $t = 0$, when heating starts, is supposed to be uniform.

A model allowing to find the temperature response $y_{mo,\,i}(t)$ of sensor number *i* (*i* = 1 to *q*) at time *t*, is sought.

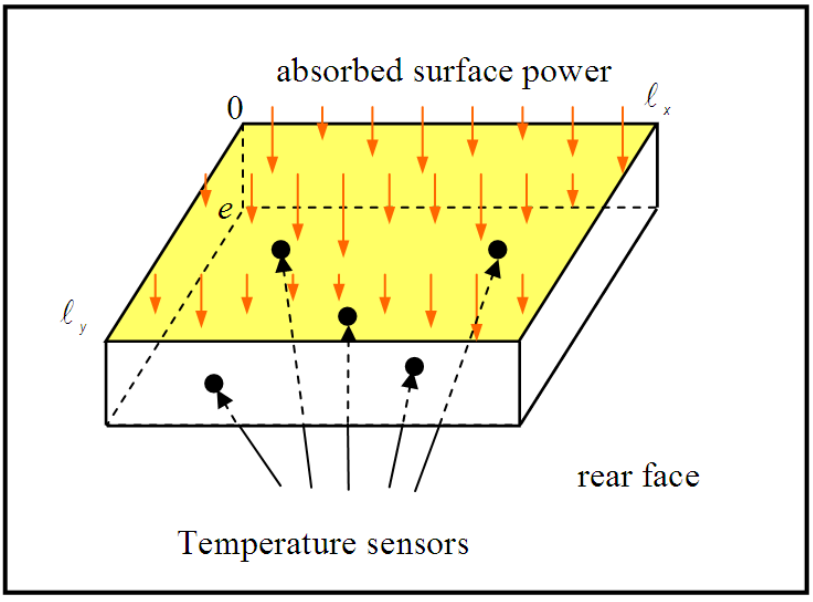

Figure 9. Model for temperature response of a slab heated on one of its faces.

a) 3D Model

Heat source *u* (*x*, *y*, *t*) (W.m^{-2}) is supposed non uniform over the front face. Evolution with time of the temperature field can be described by a three-dimension transient model, see figure 10a:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} = \frac{1}{a}\frac{\partial T}{\partial t} \tag{3.30}$$

$$T = T_0 \text{ at } \quad t = 0 \tag{3.31}$$

$$\frac{\partial T}{\partial x} = 0 \quad \text{for} \quad x = 0, \ell_x \; ; \; \frac{\partial T}{\partial y} = 0 \quad \text{for} \quad y = 0, \ell_y \tag{3.32}$$

$$-\lambda \frac{\partial T}{\partial z} = u(x, y, t) \text{ for } z = 0 \; ; \; -\lambda \frac{\partial T}{\partial z} = h\,(T - T_\infty) \quad \text{for} \quad z = e \tag{3.33}$$

This system of eight equations constitutes model $\boldsymbol{M_a}$ that will be called « detailed model », whose solution, noted $T = T_a$ here, determines the response of each sensor:

$$y_{mo,\,i} = \eta_i\,(t, x) = T_a\,(x_i,\, y_i,\, z_i\,, t\,; u\,(x, y, t),\, T_0,\, T_\infty,\, h,\, \ell_x,\, \ell_y,\, e,\, \lambda,\, a) \tag{3.34}$$

In this equation, u, T_0 and T_∞ are input quantities of the model, independent from the structure of the material system (if they are all equal to zero, temperature stay to a zero level everywhere in the slab), while the other quantities are the structural parameters $\boldsymbol{\beta}$, either linked to geometry (ℓ_x, ℓ_y, e), or to the thermophysical properties (k, a) of the slab material and to its coupling with the outside environment (h), or linked to the space location of the sensors $(x_i, y_i, z_i,$ for $i = 1$ to $q)$.

A list $x = \{\boldsymbol{\beta}, u, T_0, T_\infty\}$ can be introduced here. It gathers *structural parameters* $\boldsymbol{\beta}$, *inputs* u and T_∞ and initial state T_0, of this dynamical system composed of $(3q + 9)$ quantities.

Dimensionless 3D model

The number of quantities present in equations (3.30) and (3.33) can be reduced if they are written in a dimensionless form : dimensionless temperature $T^* = (T - T_\infty)/\Delta T$ appears, with $\Delta T = T_0 - T_\infty$, and it is the same for dimensionless time, Fourier number $t^* = a\,t/\tau_{diff}$, and dimensionless heat transfer coefficient, Biot number $H = h\,e/\lambda$. In a similar way dimensionless observation locations $x_i^* = x_i/e$, $y_i^* = y_i/e$, $z_i^* = z_i/e$ and dimensions $\ell_x^* = \ell_x/e$ and $\ell_y^* = \ell_y/e$ are introduced.

Here $\tau_{diff} = e^2/a$ is the characteristic time, related to the the duration of thermal diffusion in the thickness of the slab. The resistance of the slab in the thickness direction, related to a unit area, $R = e/\lambda$, can be introduced.

This new model $\boldsymbol{M}_a^*$ that corresponds to the same response of the sensors becomes:

$$y_{mo,i} = \eta^*(t, x^*) = \Delta T \,.\, T^*(x_i^*, y_i^*, z_i^*, t/\tau_{diff}, R,\ u(x, y, t)/\Delta T, H, \ell_x^*, \ell_y^*) + T_\infty \quad (3.35)$$

where the new list x^*, gathering the variables necessary for calculating the temperature response at a given time *t*, comprises one less parameters than the original *x* list (3.34):

$$x^* = \left\{ \boldsymbol{\beta}^*, u, \Delta T, T_\infty \right\} \text{ with } \boldsymbol{\beta}^* = ((x_i^*, y_i^*, z_i^*), \text{ for } i = 1 \text{ to } q),\ \tau_{diff},\ R, H, \ell_x^*, \ell_y^*) \quad (3.36)$$

b) 2D model in *x* and *z* directions

Model $\boldsymbol{M_a}$ can be simplified : if one knows that stimulus u does not vary much in direction *y*, or if the sensor whose response has to be simulated is not a point sensor but integrates the temperature signal in this direction, a *y*-direction average temperature field T_b can be rebuilt, with the definition of a new model $\boldsymbol{M_b}$, see figure 9b:

$$T_b(x, z, t) = \frac{1}{\ell_y} \int_0^{\ell_y} T_a(x, y, z, t)\, dy \quad (3.37)$$

This 2D temperature field is produced by a source that varies in one single space direction, instead of two previously. This new source $u_m(x, t)$ does not depend on y, and, as temperature, is the mean, in this direction, of the previous stimulus:

$$u_m(x, t) = \frac{1}{\ell_y} \int_0^{\ell_y} u(x, y, t)\, dy \quad (3.38)$$

This mean temperature field verifies the following equations:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial z^2} = \frac{1}{a} \frac{\partial T}{\partial t} \quad (3.39)$$

$$T = T_0 \text{ at } t = 0 \quad ; \quad \frac{\partial T}{\partial x} = 0 \quad \text{for } x = 0, \ell_x \quad (3.40)$$

$$-\lambda \frac{\partial T}{\partial z} = u_m(x, t) \text{ for } z = 0 \ ; \ -\lambda \frac{\partial T}{\partial z} = h(T - T_\infty) \text{ for } z = e \quad (3.41)$$

Once put in a dimensionless form, this $\boldsymbol{M_b}$ model comprises (2 q + 7) independent variables :

$$x = \left\{ \boldsymbol{\beta}, u_m, \Delta T, T_\infty \right\} \text{ with } \boldsymbol{\beta} = ((x_i^*, z_i^*, \text{ for } i = 1 \text{ to } q), \tau_{diff}, R, H, \ell_x^*) \quad (3.42)$$

Let us note now that, in order for this model to show really no bias for sensor *i*, this detector should not be a point sensor, but a line sensor.

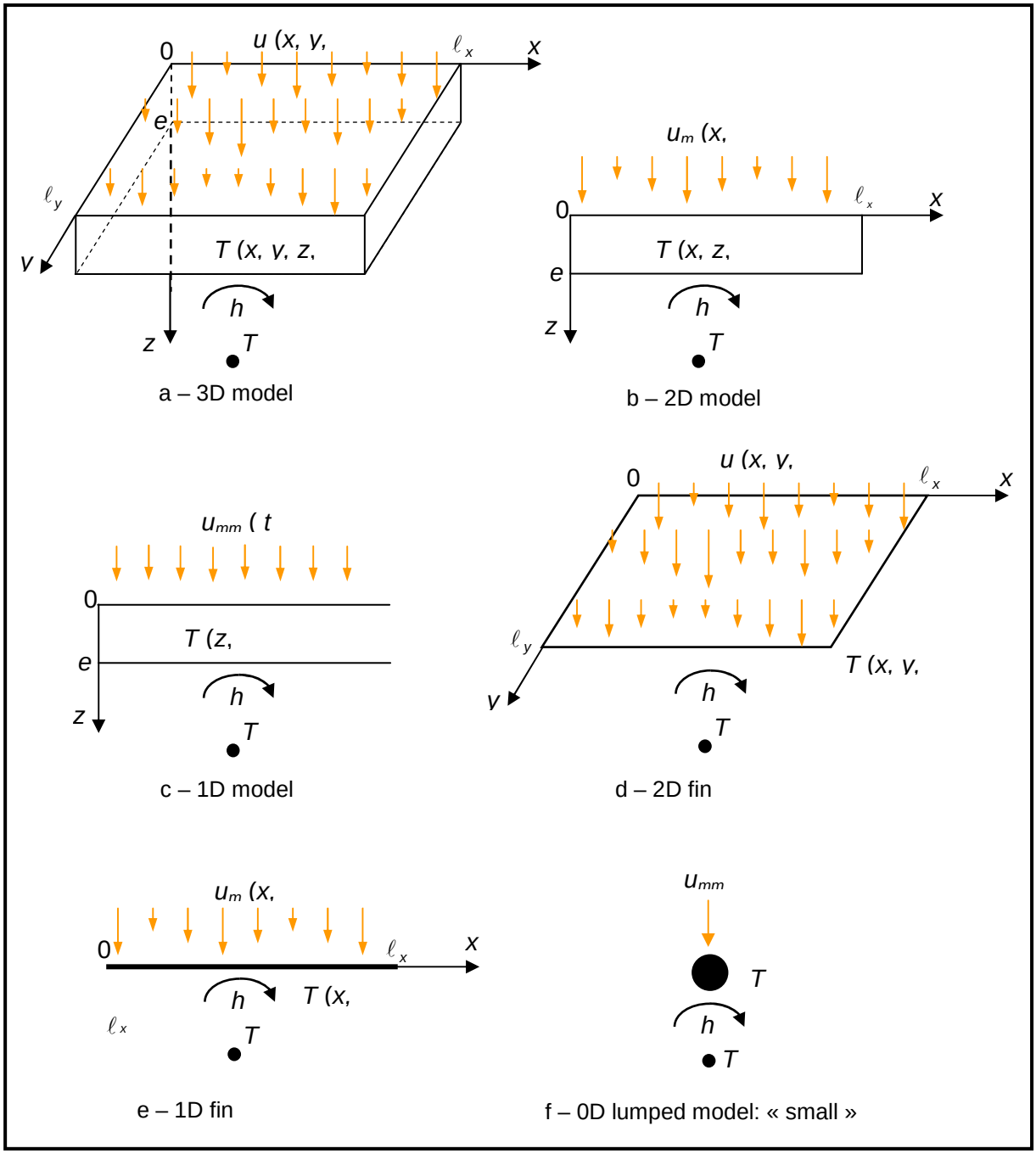

Figure 9. « Physical » model reduction

This is possible if the rear face ($z_i^* = 1$) temperature field is measured by infrared thermography. In that case output of model $\boldsymbol{M_b}$ at location (x_i, y_i), is:

$$y_{mod,i}(t_k) = T_b\ (x_i, z_i = e, t_k) \tag{3.44}$$

Its experimental counterpart can be scrutinized: one notes now $T_k^{exp}(x^m, y^j)$ the temperature signal at time t_k, for pixel (x^m, y^j) of the infrared frame, where (m, j) designates a pixel located in the m^{th} line and j^{th} column.

The output (y-averaged) temperatures of the model have to be compared with the corresponding experimental response $y_i(t_k)$ of the i^{th} detector: this can be obtained through simple addition:

$$y_i(t_k) = \frac{1}{n_i} \sum_{j=1}^{n_i} T_k^{exp}(x^m, y^j = y_i) \tag{3.45}$$

where n_i is the number of pixels in the i^{th} column (constant x^m). The reader should not be confused by the present notation in equation (3.45): $y_i(t_k)$ is the experimental temperature signal of the i^{th} detector, while y_i is its coordinate, in the y-direction).

If the average temperature in the y direction is really measured by a line sensor, there will be no model error in the estimation of $u_m(x, t)$. However, the information on the variation of u in the y direction will be lost by this reduced modelling, which means that the description of u will be made with no resolution in this direction: people in charge of this estimation would have therefore to reduce also their initial objective, that is estimation of $u_m(x, t)$ instead of $u(x, y, t)$.

c) 1D model in *z* direction

Such an averaging can be pursued if one considers now the averaged value of the source over the whole front face area. The same type of averaging is made for the temperature field. This leads to model $\boldsymbol{M_c}$, shown in figure 9c:

$$u_{mm}(t) = \frac{1}{\ell_x} \int_0^{\ell_x} u_m(x, t)\, dx \tag{3.46}$$

$$T_c(z, t) = \frac{1}{\ell_x} \int_0^{\ell_x} T_b(x, z, t)\, dx \tag{3.47}$$

$$\frac{\partial^2 T}{\partial z^2} = \frac{1}{a} \frac{\partial T}{\partial t} \tag{3.48}$$

$$T = T_0 \quad \text{for} \quad t = 0 \tag{3.49}$$

$$-\lambda \frac{\partial T}{\partial z} = u_{mm}(t) \quad \text{for} \quad z = 0\ ; \quad -\lambda \frac{\partial T}{\partial z} = h(T - T_\infty) \quad \text{for} \quad z = e \tag{3.50}$$

Once model $\boldsymbol{M_c}$ put in a dimensionless form, only (q + 6) independent variables remain in the x list:

$$x = \{ \boldsymbol{\beta}, u_{mm}, \Delta T, T_\infty \} \quad \text{with} \quad \boldsymbol{\beta} = ((z_i^*, \text{ for } i = 1 \text{ to } q), \tau_{diff}, R, H) \tag{3.51}$$

This reduction in the number of variables is made at the expense of the space resolution for u, that is completely lost here since it is replaced by its space average u_{mm} .

d) 2D Fin model in *x* and *y* directions

If the Biot number $H = he/k$ is much lower than unity, temperature variations in the z direction, corresponding to the slab thickness, can be considered as two-dimensional. The resulting 2D temperature field stems from an integration, with respect to z, of the 3D temperature field, see figure 9d:

$$T_d\ (x, z, t) = \frac{1}{e} \int_0^e T_a\ (x, y, z, t)\ \mathrm{d}z \tag{3.52}$$

This reduced model $\boldsymbol{M_d}$ corresponds to a 2D fin whose temperature verifies the following equations :

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} - \frac{h\ (T - T_\infty)}{\lambda e} + \frac{u\ (x, y, t)}{\lambda e} = \frac{1}{a} \frac{\partial T}{\partial t} \tag{3.53}$$

$$T = T_0 \quad \text{at} \quad t = 0 \tag{3.54}$$

$$\frac{\partial T}{\partial x} = 0 \quad \text{for} \quad x = 0, \ell_x \ ; \ \frac{\partial T}{\partial y} = 0 \quad \text{for} \quad y = 0, \ell_y \tag{3.55}$$

List x is now composed of (2 q + 8) independent variables :

$$x = \{ \boldsymbol{\beta}, u, \Delta T, T_\infty \} \text{ with } \boldsymbol{\beta} = ((x_i^*, y_i^*, \text{ for } i = 1 \text{ to } q), \tau_{diff}, R, H, \ell_x^*, \ell_y^*) \tag{3.56}$$

This relatively high number of variables allows however to keep the initial spatial resolution of stimulus u.

e) 1D fin model in *x* direction

The 2D reduced model $\boldsymbol{M_b}$ can be used now to construct a 1D fin model, noted $\boldsymbol{M_e}$, with the same condition on the Biot number H, through an integration in the z direction (the same model $\boldsymbol{M_e}$ can be obtained trough integration of model $\boldsymbol{M_d}$ in y direction), see figure 9e:

$$T_e\ (x, t) = \frac{1}{e} \int_0^e T_b\ (x, z, t)\ \mathrm{d}z \tag{3.57}$$

$$\frac{\partial^2 T}{\partial x^2} - \frac{h\,(T - T_\infty)}{\lambda e} + \frac{u_m\,(x, t)}{\lambda e} = \frac{1}{a}\,\frac{\partial T}{\partial t} \tag{3.58}$$

$$T = T_0 \quad \text{at} \quad t = 0 \tag{3.59}$$

$$\frac{\partial T}{\partial x} = 0 \quad \text{for} \quad x = 0,\ \ell_x \tag{3.60}$$

List x of the independent variables of the model is composed of (q + 7) quantities:

$$x = \{\boldsymbol{\beta},\, u_m,\, \Delta T,\, T_\infty\} \quad \text{with} \quad \boldsymbol{\beta} = ((z_i^*, \text{ for } i = 1 \text{ to } q),\, \tau_{diff},\, R,\, H) \tag{3.61}$$

f) 0D lumped model

If the source is nearly uniform in space, with a low Biot number in direction z, or if the sensor provides the volume averaged temperature of the slab, one obtains a 0D $\boldsymbol{M_f}$ model, also called lumped model or « small body » model. It corresponds to integration of model $\boldsymbol{M_e}$ in the x direction, see figure 9f:

$$T_f\,(t) = \frac{1}{\ell_x}\int_0^e T_e\,(x, t)\,\mathrm{d}x \tag{3.62}$$

This temperature field is produced by a point source whose intensity $u_{mm}(t)$ varies with time, with :

$$u_{mm}(t) = \frac{1}{\ell_x}\int_0^{\ell_x} u_m\,(x,\, t)\,\mathrm{d}x \tag{3.63}$$

The heat equation becomes :

$$\rho c e\,\frac{\mathrm{d}T}{\mathrm{d}t} + h\,(T - T_\infty) = u_{mm}\,(t) \tag{3.64}$$

with:

$$T = T_0 \quad \text{at} \quad t = 0 \tag{3.65}$$

The x list of this model is now composed of only 5 independent variables, including a convective resistance (based on a unit area) G = 1/h and a time constant $\tau = \rho c e / h = \tau_{diff} / H$:

$$x = \{\boldsymbol{\beta},\, u_{mm},\, \Delta T,\, T_\infty\} \quad \text{with} \quad \boldsymbol{\beta} = (\tau, G) \quad \text{and} \quad \Delta T = T_0 - T_\infty \tag{3.66}$$

An analytical solution can easily be found :

$$T = T_\infty + \Delta T\ exp\ (-t / \tau) + \frac{G}{\tau}\int_0^t u_{mm}(t')\,\exp\left(-\frac{t - t'}{\tau}\right)\mathrm{d}t' \tag{3.67}$$

This model is a limit model, only valid if the Biot number, based on the largest of the three dimensions ℓ_x, ℓ_y or e, is much lower than unity. If not, it is a biased model, but its output T_f can always be compared to the average temperature of the q sensors. This averaged experimental temperature brings an interesting information on the time variation of the average absorbed power density on the front face, $u_{mm}(t)$.

g) 1D local model

A last model, noted $\boldsymbol{M_g}$ here, can be used. It is a 1D « local » temperature defined by:

$$y_{mo,i} = T_g(x_i, y_i, t) = T_c(z_i, t\ ;\ u(x_i, y_i, t), \Delta T, T_\infty, \boldsymbol{\beta}) \tag{3.67}$$

with

$$\boldsymbol{\beta}_i = (z_i^*, \tau_{diff\ i}, R_i, H_i) \tag{3.68}$$

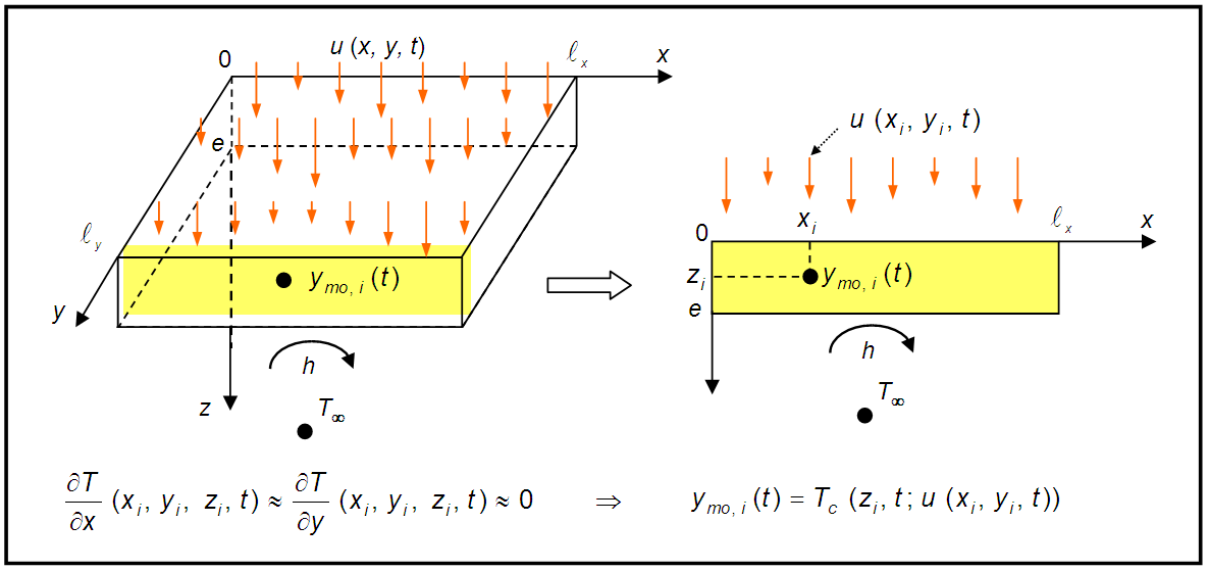

Figure 10. 1D local model *Mg*

It corresponds to the previous 1D model $\boldsymbol{M_c}$, applied locally for each sensor. Its response depends on the sole excitation $u(x_i, y_i, t)$ that prevails on the front face at the same (x, y) location, see figure 10.

This allows to consider a 3D problem as a set of independent 1D problems, each individual problem being associated to a specific sensor. Structural parameters belonging to vector $\boldsymbol{\beta}_i$ differ for each sensor. This vector is composed of a diffusion characteristic time $\tau_{diff\ i}$, a resistance R_i and a Biot number H_i, that have all local values corresponding to location of sensor i. These structural parameters are related to local thickness e_i, local heat transfer coefficient h_i, and local conductivity k_i and diffusivity a_i.

For the whole set of sensors, this model is composed of (q + 6) independent variables if these sensors are embedded at the same depth in the slab and if the thermophysical parameters, h, and the slab thickness do not varry in the x – y plane.

This model is valid only if heat transfer is negligible in the directions of this same plane, that is if the slab is made of a composite material that is homogenized but anisotropic : the principal directions of conductivity tensor $\overline{\overline{k}}$ shoud be those of the slab, with principal components $k_x = k_y = 0$, $k_z = k$. However, it is possible to use it with a reasonable bias for sensors facing front face locations where stimulus u does not vary much (low gradient in the plane of this face) and for low thickness and thermophysical local variations. This model is also very interesting in non destructive testing of composite slabs by infrared thermography [9].

Remarks

- The six reduced models $\boldsymbol{M_b}$ to $\boldsymbol{M_g}$ are all derived from the detailed model $\boldsymbol{M_a}$ and have lower dimensions than this original 3D model. They are also characterized by a lower number of structural parameters.

- Structural parameters of the slab and of the sensors either disappear or are transfered from one model to a more reduced one along this progressive physical reduction process. So passing from model $\boldsymbol{M_e}$ to model $\boldsymbol{M_f}$ makes parameter ℓ_x^* , R and x_i^* disappear while parameters H and τ_{diff} merge into a single parameter $\tau = \tau_{diff} / H$. This reduction of the parameters number is an irreversible one, which means that it is not possible to rebuild values of H and τ_{diff} starting from the knowledge of τ only.

- One can also note that during this reduction process, relationships between former and new parameters are linear if the logarithms of these parameters are considered: $\ln(\tau) = \ln(\tau_{diff}) - \ln(H)$. This gives an interesting relationship between reduced sensitivities (see also lecture 4 in this school).

- In parallel with the reduction in the number of parameters, a reduction of the space dimension necessary for reproducing the sensors behaviour appears : from an initial $u(x, y, t)$ stimulus for models $\boldsymbol{M_a}$ and $\boldsymbol{M_d}$, one gets a $u_m(x, t)$ stimulus for models $\boldsymbol{M_b}$ and $\boldsymbol{M_e}$ to finally $u_{mm}(t)$ for models $\boldsymbol{M_c}$ and $\boldsymbol{M_f}$ and $u_i(t) = u(x_i, y_i, t)$ for model $\boldsymbol{M_g}$.

- All these models rely on specific physical assumptions and none of them corresponds to the absolute reality, even model $\boldsymbol{M_a}$: this one neglects convecto-radiative losses on the front face and on the four sides of the slab, coefficient h is supposed uniform in the rear face plane and the same is true for the initial temperature inside the slab.

This example shows that the user has to make its own choice for the model, since several representations are generally possible. Accordingly a more reduced model conveys less information about the spatial distribution of the heat source. However, this inconvenient in direct modelling can become an asset when inversion, to reconstruct the source, takes place.

4. Conclusion

The aim of this lecture, located right after lecture 2, which deals with inversion related to generic linear models, was to introduce the notion of model associated with measurements in a physical system subjected to heat transfer. Whatever the situation, the model-builder has a given objective (thermophysical characterization, heat flux estimation, system identifiication, …) and is free to construct a model adapted both to his needs and to his constraints (lack of information, partial measurements, …). This model can be of the white, grey of black box type. It requires the definition of a large number of quantities (parameters or functions, input and observations, explanatory variables) that must be either discretized or parameterized.
In a similar way and in parallel, measurements coming from sensors require the construction of a calibration law (a specific inverse problem) and introduce a noise that will be one of the causes (but not the only one) of the estimation errors.

In order to prevent the ill-conditioning of the corresponding inverse problem, special care has to be given for both measurements (non intrusive) and to model. Models used for inversion differ from models used for simulation: they should have a minimum number of parameters (see the concept of *number of degrees of parametric freedom* in lecture 4 of this school), which means that parcimony is a plus and model reduction, for example on a physical basis, can bring more stability to the subsequent inversion. Interested readers can refer to references [1], 10] and [11] for more insight on this subject.

References

[1] *Thermal Measurements and Inverse Techniques*, Editors**:** Helcio R.B. Orlande; Olivier Fudym; Denis Maillet; Renato M. Cotta, Publisher: CRC Press, Taylor & Francis Group, Bocca Raton, USA, 779 pages, May 09, 2011

[2] Ozisik, M.N. . 1980. *Heat conduction*. Chichester: Wiley.

[3] Maillet, D., S. André, J.C. Batsale, A. Degiovanni, C. Moyne. 2000. *Thermal Quadrupoles – Solving the Heat Equation through Integral transforms*. Wiley: Chichester.

[4] Press, W.H., Flannery (B.P.), Teulkosky, S.A., Vetterling, W.T. 1992. *Numerical Recipes - The Art of Scientific Computing*, New York: Cambridge University Press.

[5] Testu, A., S. Didierjean, D. Maillet, C. Moyne, T. Metzger, T. Niass. 2007. Thermal dispersion coefficients for water or air flow through a bed of glass beads. *Int. J. Heat and Mass Transfer*, vol. 50, Issues 7-8 (April): 1469-1484.

[6] Maillet, D. A.S. Houlbert, S. Didierjean, A.S. Lamine and A. Degiovanni. 1993.
Nondestructive thermal evaluation of delaminations inside a laminate - Part I: Identification using the measurement of a thermal contrast and Part II: The experimental Laplace

transforms method. *Composites Science and Technology*, vol. 47 , no. 2 :137-154 and 155-172.

[7] Rémy, B. A. Degiovanni. 2005. Parameters estimation and measurement of thermophysical properties of liquids. *International Journal of Heat and Mass Transfer*, volume 48, nos. 19-20 (September) 2005: 4103-4120

[8] Girault, D. Maillet, F. Bonthoux, B. Galland, P. Martin, R. Braconnier, J.-R. Fontaine. 2008. Estimation of time-varying pollutant emission rates in a ventilated enclosure: inversion of a reduced model obtained by experimental application of the Modal Identification Method. *Inverse Problems*, vol. 24, Issue 1 February), 01 5021, 22 pages.

[9] Benítez, H.D, Ibarra-Castanedo, C., Bendada, A., Maldague, X., Loaiza, H., Caicedo, E.. 2008. Definition of a new thermal contrast and pulse correction for defect quantification in pulsed thermography. *Infrared Physics and Thermography*, volume 51, no. 3 (January): 160-167.

[10] D. Petit, D. Maillet, Techniques inverses et estimation de paramètres (Inverse techniques and parameter estimation), Editeur: Techniques de l'Ingénieur, thème : Sciences Fondamentales, base : Physique-Chimie, rubrique : Mathématiques pour la physique, dossiers AF 4515, pp. 1- 18, et AF 4516, pp. 1-24, Paris, janvier 2008.

[11] D. Maillet, Y. Jarny, D. Petit, Problèmes inverses en diffusion thermique (Inverse Problems in thermal diffusion), Dossiers BE 8265 "Modèles diffusifs, mesures et introduction à l'inversion" (Diffusive models and introduction to inversion), pp. 1- 54, octobre 2010,
BE 8266 "Formulation et résolution du problème des moindres carrés" (Formulation and solution of the least squares problem", pp. 1-46, janvier 2011, and BE 8267 "Outils spécifiques de conduction inverse et de régularisation" (Specific tools for inverse conduction and regularization), pp. 1-46, July 2011, Techniques de l'Ingénieur, Paris, base documentaire: Génie Energétique.