MODELING AND SIMULATION OF DISTRIBUTED PARAMETER SYSTEMS

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Contents

Summary

Distributed parameter systems are modeled by sets of partial differential equations, boundary conditions and initial conditions, which describe the evolution of the state variables in several independent coordinates, e.g. space and time. Most distributed parameter models are derived from first-principles, i.e. conservation of mass, energy and momentum.

Whereas first-principles allow a model structure to be defined, some degrees of freedom are usually left for model parameterization, and a number of unknown parameters have to be estimated from experimental data by minimizing an output error criterion measuring the deviation between real system and model outputs. At this stage, experiment design, sensor configuration, and measurement errors are important issues, which have to be considered in order to ensure parameter identifiability.

In addition, model reduction techniques, based on simplifying assumptions regarding the problem physics, dimensionality and geometry, and based on various techniques including parameter sensitivity analysis and singular perturbations, are also very useful in deriving a model suitable for control, i.e. a model compromising complexity and efficiency in reproducing the major physical phenomena.

Once a distributed parameter model has been obtained, a system simulator can be implemented. Due to the inherent complexity and nonlinearity of the model equations, an analytical solution is usually intractable, and it is necessary to resort to a numerical procedure. One of the most popular approaches is the numerical method of lines, which proceeds in two basic steps: (a) spatial approximation and (b) time integration. A vast array of numerical algorithms are available, either for spatial approximation, e.g. weighted residual, finite element, finite difference and finite volume methods, or for time integration, e.g. explicit and implicit solvers with variable steps, adjustable order of accuracy and sophisticated matrix algebra.

These latter numerical approximation techniques can be exploited at two different stages for control purposes: (a) the early lumping approach, in which the distributed parameter model is first reduced to a lumped parameter system and conventional control schemes are then applied, and (b) the late lumping approach, in which the distributed nature of the system is kept along the control design procedure, and numerical approximation techniques are used at a final stage only, to approximate the resulting partial differential Eqs. (describing state estimation/control) for real-time implementation.

1. Introduction

Many systems from science and engineering are distributed parameter systems (DPSs), i.e. systems characterized by state variables (or dependent variables) in two or more coordinates (or independent variables). Time and space is the most frequent combination of independent variables, as is the case in the following examples:

- time-varying temperature profiles in a heat exchanger,
- time-varying concentration profiles in a sorptive packed column,
- time-varying temperature and concentration profiles in a tubular reactor,
- time-varying car density along a highway,
- time-varying deflection profile of a beam subject to external forces,
- time-varying shape and velocity of a water wave,

but other combinations of independent variables are possible as well. For instance, time and individual size (or another characteristic such as age) occur in population models used in ecology, or to describe some important industrial processes such as polymerization, crystallization or material grinding. In these models, space can also be required to represent the distribution of individuals (of various sizes) in a spatial region or in a non homogeneous reactor medium (due to non ideal mixing conditions in a batch reactor, or to continuous operation in a tubular reactor).

The preceding examples show that there exists a great variety of DPSs, arising from different areas of science and engineering, which are characterized by time-varying

distributions of dependent variables. In view of the system complexity, a mathematical model, i.e. a mathematical description of the physical (chemical, mechanical, electrical, etc.) phenomena taking place in the system, is often a prerequisite to system analysis and control. Such a model consists of partial differential Eqs. (PDEs), boundary conditions (BCs), and initial conditions (ICs) describing the evolution of the state variables. In addition, DP systems can interact with lumped parameter systems (LPSs), whose state variables are described by ordinary differential Eqs. (ODEs), and supplementary algebraic model equations can be used to express phenomena such as thermodynamic equilibria, heat and mass transfers and reaction kinetics.

Hence, a DPS is usually described by a mixed set of nonlinear PDEs/ODEs/AEs or PDAEs. For control purposes, it is also required to select input and output variables, and to define the associated equations. Thereby, process disturbances are assumed to be known or to be modeled by additional equations. Most PDAE models are derived from first-principles, i.e. conservation of mass, energy and momentum, and are given in a state space representation which is the basis for system analysis and control.

Whereas first-principles and physical laws allow a model structure to be defined, some degrees of freedom are available when selecting the model parameterization, and a number of unknown parameters have to be inferred from experimental data. This latter task can be achieved by minimizing an output error criterion measuring the deviation between real system and model outputs. At this stage, experiment design, sensor configuration, and measurement errors are important issues, which have to be considered in order to ensure parameter identifiability.

In addition, model reduction techniques, based on simplifying assumptions regarding the problem physics, dimensionality and geometry, and based on various techniques including parameter sensitivity analysis and singular perturbations, are also very useful to derive a model suitable for model-based control, i.e. a model compromising complexity and efficiency in reproducing the major physical phenomena.

Once a DP model has been obtained, the next natural step is the implementation of a system simulator. Due to the inherent complexity and nonlinearity of the PDAE model, an analytical solution is usually intractable, and it is necessary to resort to a numerical procedure. One of the most popular approaches is the numerical method of lines (MOL), which proceeds in two basic steps:

- approximation of the spatial derivatives using finite differences, elements or volumes;
- time integration of the resulting semi-discrete (discrete in space – continuous in time) system of equations, which takes the form of algebro-differential Eqs. (DAEs).

The MOL has received considerable attention in the last decades and a vast array of numerical algorithms for spatial approximation and time integration are now available.

The DP model, and associated simulator, can then be used to analyze the system dynamics and to design controllers. Due to the infinite order of DPSs, two main

approaches can be taken:

- the early lumping approach, in which the model partial differential equations are approximated (lumped) first, and the control design proceeds with the lumped model equations. The approximation technique is usually selected with the concern of dimensionality, as control design requires manipulation of the model equations, and polynomial approximations, such as orthogonal collocation, have been central to numerous developments;
- the late lumping approach, in which the distributed nature of the system is kept as long as possible in the course of the control design. In the end, computer implementation of the resulting control algorithms requires numerical approximation techniques. However, dimensionality is no longer critical, as no further analytical manipulation of the equations are required. Of course, accuracy and computational load are important issues.

This chapter is all about the preceding ideas and attempts to present an informative overview of existing modeling and simulation techniques for DPSs. The text is organized as follows.

Section 2 deals with modeling of DPSs. First, Section 2.1. introduces the PDE formalism and the methodology used to derive DP models. Several classifications of PDEs and BCs are presented in Section 2.2. The parameter estimation problem in DPSs is addressed in Section 2.3, and model simplification/reduction techniques are discussed in Section 2.4.

After this introduction to DPS modeling, analytical and numerical solution procedures are presented in Section 3. Particularly, attention is focused on the method of separation of variables and eigenfunction expansions in Section 3.1. Then, Section 3.2. describes weighted residual methods, and Section 3.3. deals with spatial discretization, i.e. finite element, difference and volume methods. Some important aspects of time integration are addressed in Section 3.4, and finally, Section 3.5 discusses early and late lumping approaches to control design.

2. Modeling of Distributed Parameter Systems

DPSs are described by nonlinear PDAEs, which are derived from first-principles, e.g. mass, energy and momentum balances. Even though the physical model formulation can involve higher-order time derivatives (e.g. the wave equation, which is used to describe the motion of a string, is second-order in time), it is straightforward to reformulate the equations in a state space representation (involving first-order time derivatives only) through a change of variables. This state space representation is the preferred form for analysis and control purposes, as well as for a numerical solution using the method of lines. In compact form, the coupled PDAEs read

$$\mathbf{M}(t,\mathbf{z},\mathbf{x})\,\mathbf{x}_t = \mathbf{f}(t,\mathbf{z},\mathbf{x},\mathbf{u},\mathbf{x}_z,\mathbf{x}_{zz},\ldots) \qquad \mathbf{z}\in\Omega \qquad (1)$$

$$\mathbf{0} = \mathbf{g}(t,\mathbf{z},\mathbf{x},\mathbf{v},\mathbf{x}_z,\ldots) \qquad \mathbf{z}\in\Gamma \qquad (2)$$

$$\mathbf{x}(t=0,\mathbf{z}) = \mathbf{x}_0(\mathbf{z}) \qquad \mathbf{z} \in \Omega \cup \Gamma \qquad (3)$$

where Eq. (1) can, in general, include PDEs defined in the spatial domain Ω, as well as ODEs and AEs. In turn, the presence of algebraic relationships in (1) involves a singular mass matrix $\mathbf{M}$ (i.e. $\mathbf{M}$ has a null line corresponding to each algebraic state in the vector $\mathbf{x}$). The PDEs are supplemented by BCs (2) at the boundary surface Γ and ICs (3) (which also include the ICs required for the model ODEs, if any). In these expressions, $\mathbf{x}_t = \partial\mathbf{x}/\partial t$, and $\mathbf{x_z}$ and $\mathbf{x_{zz}}$ represent first- and second-order partial derivatives of the state $\mathbf{x}(t,\mathbf{z})$ with respect to the spatial coordinate $\mathbf{z} = (z_1, z_2, z_3)$. In (1), $\mathbf{f}$ is a vector of nonlinear functions of the state and several of its spatial derivatives as well as of the input $\mathbf{u}(t,\mathbf{z})$ acting in the spatial domain Ω. At the boundary surface Γ, the balance equations reduce to algebraic BCs (2), which involve boundary inputs $\mathbf{v}(t,\mathbf{z})$.

2.1. Model Derivation – Basic Principles

The model equations are derived from application of first principles, i.e. conservation of mass, energy and momentum. If any of these quantities is denoted by *x*, the following general balance equation can be written

$$\begin{aligned} &\textit{Accumulation of } x \;\; = \textit{flow of } x \textit{ in} - \textit{flow of } x \textit{ out} \\ &\qquad\qquad + \textit{amount of } x \textit{ generated} - \textit{amount of } x \textit{ consumed} \end{aligned} \qquad (4)$$

To illustrate this general principle, a specific example is considered, namely the adsorption of a chemical component in a packed bed column (Fig. 1)

An incompressible liquid phase containing a chemical component *C* enters into the column with a concentration $c_l(t, z=0) = c_{l,\text{in}}(t)$. The fluid flows through the solid particles of the bed, where the chemical component *C* can be adsorbed or desorbed. It is assumed that there is no radial gradient of concentration, so that the two independent variables are the time *t* and the spatial coordinate along the column *z*. The concentrations of *C* in the liquid phase $c_l(t,z)$ and in the solid phase $c_s(t,z)$ are the dependent variables (or state variables) of the system. The PDEs describing the space-time evolution of these state variables are obtained by expressing mass balances in the form of (4) for an elementary volume $A\Delta z$ of the column (see Fig. 1), i.e.

$$A\varepsilon\Delta z\left(c_l(t+\Delta t,z) - c_l(t,z)\right) = A\varepsilon v c_l(t,z)\Delta t - A\varepsilon v c_l(t,z+\Delta z)\Delta t - A\varepsilon\Delta z\Phi_{\text{ads}}\Delta t \quad (5)$$

$$A(1-\varepsilon)\Delta z\left(c_s(t+\Delta t,z) - c_s(t,z)\right) = 0 - 0 + A\varepsilon\Delta z\Phi_{\text{ads}}\Delta t \qquad (6)$$

where *A* is the cross-section area of the column, ε is the void fraction (porosity of the solid bed), *v* is the intersticial velocity of the fluid and Φ_{ads} is the adsorption flux, which can be expressed in several ways. Here, a linear driving force model is used

$$\Phi_{\text{ads}}(t,z) = k(q(t,z) - c_s(t,z)) \qquad (7)$$

where $q(t,z)$ is the equilibrium concentration of the adsorbed component at the solid interface, which can be described by various adsorption isotherms, e.g. a Freundlich isotherm in the form

$$q(t,z) = \alpha\, c_l^{\beta}(t,z) \tag{8}$$

Dividing both sides of Eqs. (5-6) by $\Delta t \Delta z$, letting $\Delta t \to 0$, $\Delta z \to 0$ and rearranging the several terms lead to

$$\frac{\partial c_l}{\partial t} = -v\frac{\partial c_l}{\partial z} - \Phi_{\text{ads}} \qquad z \in (0, L) \tag{9}$$

$$\frac{\partial c_s}{\partial t} = +\frac{\varepsilon}{(1-\varepsilon)}\Phi_{\text{ads}} \tag{10}$$

Equation (9) is a first-order PDE, which has to be supplemented by one BC at the column inlet

$$c_l(t, z=0) = c_{l,\text{in}}(t) \tag{11}$$

and one IC

$$c_l(t=0, z) = c_{l,0}(z) \qquad z \in [0, L] \tag{12}$$

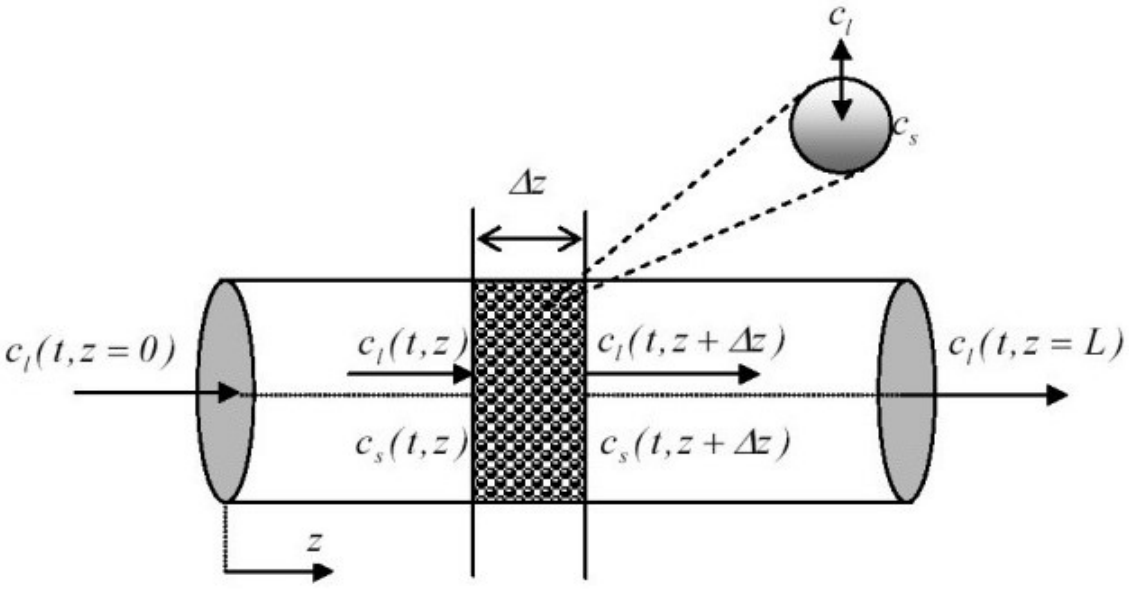

Figure 1. Adsorption of a chemical component in a packed bed column

If dispersion in the particle bed is taken into account, then additional material transportation terms are added to the right-hand side of (5), i.e.

$$-A\varepsilon D\left.\frac{\partial c_l}{\partial z}\right|_{(t,z)}\Delta t + A\varepsilon D\left.\frac{\partial c_l}{\partial z}\right|_{(t,z+\Delta z)}\Delta t \tag{13}$$

where D is the axial dispersion coefficient.

In this case, (9) becomes a second-order PDE

$$\frac{\partial c_l}{\partial t} = -v\frac{\partial c_l}{\partial z} + D\frac{\partial^2 c_l}{\partial z^2} - \Phi_{\text{ads}} \qquad z \in (0, L) \tag{14}$$

which requires a second boundary condition, e.g.

$$\left.\frac{\partial c_l}{\partial z}\right|_{(t,z=L)} = 0 \tag{15}$$

expressing that dispersion is negligible at the column outlet.

On the other hand, the mass balance (10) for the solid phase is a PDE without spatial derivatives, as there is no solid movement. Hence, this equation just require an IC of the form

$$c_{\text{s}}(t=0,z) = c_{\text{s},0}(z) \qquad z \in [0, L] \tag{16}$$

Note that, if the adsorption dynamics is very fast, a quasi steady-state assumption for the solid phase can be made, i.e. the concentration in the solid phase is at the equilibrium concentration

$$c_{\text{s}}(t,z) = q(t,z) \qquad z \in [0, L] \tag{17}$$

In this latter case, PDE (14) (or 9) can be reformulated in a slightly different form

$$\frac{\partial c_l}{\partial t} + \frac{1-\varepsilon}{\varepsilon}\frac{\partial c_s}{\partial t} = -v\frac{\partial c_l}{\partial z} + D\frac{\partial^2 c_l}{\partial z^2} \qquad z \in (0, L) \tag{18}$$

The model (8, 11-12, 15, 17-18) is a mixed PDE/AE system, which illustrates the concept of mass matrix in Eq. (1) (here the mass matrix $\mathbf{M} = \begin{bmatrix} 1 & (1-\varepsilon)/\varepsilon \\ 0 & 0 \end{bmatrix}$ for the vector of state variables $x = \begin{bmatrix} c_l \\ c_{\text{s}} \end{bmatrix}$). Alternatively, (17) could be substituted into (18), thus reducing to a single PDE for $c_l(t,z)$. These several model forms correspond to different modeling assumptions (adsorption described by a linear driving force model or by an equilibrium model) and different levels of algebraic manipulation.

Most mathematical models can be obtained following these lines of thoughts, expressing mass, energy and momentum balances, and using physical, chemical, mechanical,

electrical algebraic relationships or experimental correlations. Note, at this stage, that source terms like the adsorption kinetics (7, 8), can be very delicate to model in practice as they represent phenomena that are by far more complex than their usual mathematical representations let suppose (other examples of this inherent complexity can be found in biology, where extremely complex reaction pathways are represented by simple macroscopic reaction schemes and kinetics, e.g. Monod, Haldane, etc.). This observation has led to the development of hybrid physical-black box models, such as the hybrid first-principles-neural-network models recently proposed in the specialized literature.

Modeling, however, remains much of an art, and besides the main guidelines given in this section, the experience and skills of the modeler play an important role.

2.2. More PDEs – Classifications

After having introduced the basic principles of DP modeling, the aim of this section is to review the main classes of PDEs and BCs, and to introduce various classifications.

There are basically three mathematical features that allow PDEs to be classified: order, (non)linearity and geometric consideration (elliptic, parabolic and hyperbolic PDEs).

2.2.1. PDE order

The order of a PDE is the order of its highest derivative. For example, PDE (9) is first-order in time and first-order in space, whereas PDE (14) is second-order in space. The order of a PDE determines the number of ICs and BCs that are required to completely define the initial-boundary value problem (IBVP). PDE (9) requires one IC given by (12) and one BC given by (11), whereas PDE (14) requires two BCs given by (11) and (15).

2.2.2. Linearity, Quasilinearity and Nonlinearity

When the dependent variables and their derivatives appear in linear combinations, then the PDE model is linear. Linearity is an ideal characteristic, which is unfortunately seldom present in engineering processes. Whereas there exists a complete array of analytical methods for analysis and control of linear DPSs, there exists no such comprehensive theoretical treatment for nonlinear PDEs, and it is then necessary to resort to numerical techniques. A special class of nonlinear systems is sometimes distinguished, for which more theoretical results are available: the quasilinear PDEs in which the highest derivative appears in linear form (but not necessarily the lower-order terms).

2.2.3. Elliptic, parabolic and hyperbolic PDEs

This classification is based on the second-order quasilinear formulation

$$a(\eta,\xi)x_{\eta\eta} + 2b(\eta,\xi)x_{\eta\xi} + c(\eta,\xi)x_{\xi\xi} = f(\eta,\xi,x,x_{\eta},x_{\xi}) \tag{19}$$

where η and ξ can be any of t, z_1, z_2, z_3.

If $b^2 - ac < 0$, the equation is elliptic, e.g. Poisson's equation $\frac{\partial^2 x}{\partial z_1^2} + \frac{\partial^2 x}{\partial z_2^2} = f(z_1, z_2)$.

If $b^2 - ac = 0$, the equation is parabolic, e.g. the heat Eq. (Fourier's equation) $\frac{\partial x}{\partial t} = \lambda \frac{\partial^2 x}{\partial z^2}$.

If $b^2 - ac > 0$, the equation is hyperbolic, e.g. the wave equation $\frac{\partial^2 x}{\partial t^2} = c^2 \frac{\partial^2 x}{\partial z^2}$.

However, this latter classification is of little use in engineering practice, and another, more physical, classification can be more appealing.

2.2.4. Convection - Diffusion (Dispersion) – Reaction PDEs

First-order terms (involving x_z) are representative of convective transport, whereas second-order terms (involving x_{zz}) represent diffusion and/or dispersion phenomena. The distinction between these two transportation mechanisms is fundamental in system analysis (convection corresponds to the transport of information in a "plug flow" manner, whereas diffusion/dispersion has no preferential direction, and influences all the spatial domain at the same time) and in the selection of numerical algorithms for the approximation of spatial derivatives (approximation schemes have to take account of the nature/direction of the transport phenomena). Besides convective and diffusive terms, PDEs can include source terms (separate terms in the dependent and/or independent variables), which represent various internal phenomena such as reaction, adsorption (as in PDEs 9 and 14), grinding, etc. For simplicity, these source terms are referred here as "reaction". They often represent the major sources of nonlinearity in the process model (and can be delicate to formulate/identify in practice).

2.2.5. Boundary conditions

As already mentioned in several places, a number of BCs are required to completely specify an IBVP. These BCs can belong to three main categories:

- *Dirichlet BCs* impose the value of the dependent variable at the boundary surface, i.e.

$$\mathbf{x} = \mathbf{q}(t, \mathbf{z}) \qquad \mathbf{z} \in \Gamma \qquad (20)$$

  In the example of the adsorption column (Section 2.1), (11) is a Dirichlet BC.

- *Neumann BCs* impose the value of the flux (normal to the boundary surface), i.e.

$$\frac{\partial \mathbf{x}}{\partial \mathbf{n}} = \mathbf{q}(t, \mathbf{z}) \qquad \mathbf{z} \in \Gamma \qquad (21)$$

  In the adsorption column, (15) is a Neumann BC.

- Mixed BCs are combinations of the previous BCs. For the adsorption column model (14), (11) could be replaced by a more general condition (e.g. Danckwerts boundary conditions)

$$vc_{l,\text{in}}(t) = vc(t, z=0) - D\left.\frac{\partial c}{\partial z}\right|_{t,z=0} \tag{22}$$

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Biographical Sketch

Alain Vande Wouwer was born in Ixelles, Belgium, in 1966. He graduated in electrical engineering from the Faculté Polytechnique de Mons in 1988 and received the European doctorate degree in 1994 (Faculté Polytechnique de Mons-Stuttgart University). In 1994, he achieved a post-doctoral stay in the Mechanical Engineering Department at Laval University, Quebec. Presently, he is Associate Professor in the Control Department of the Faculté Polytechnique de Mons. His research interests are in distributed parameter systems, parameter and state estimation, and bioprocess control.