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IFAC-PapersOnLine 48-13 (2015) 150–153

Dissipative boundary control systems with application to an isothermal tubular reactor ⋆

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Abstract: In this discussion paper we present two different parametrizations of the differential operator and their associated closure relations describing a model of an isothermal tubular reactor. From these two parametrizations we derive the boundary port variables of the system and check the existence of solutions in the case of Dankwert boundary conditions. We show that existence of solution can be derived from both the coercivity condition on the closure relations and some inequality condition on the input matrix mapping. Even if in the case of constant parameters these two approaches are equivalent, the canonical factorization is the only one that can be applied when some of the parameters depends on the spatial variable. This property is of major interest when linearized non isothermal tubular reactors are considered.

Keywords: Port Hamiltonian Systems, Distributed Systems, Irreversible Thermodynamics

1. INTRODUCTION

The aim of this paper is to discuss the impact of the parametrization of 1D linear differential operators on the analysis of solutions of the associated PDE systems. The discussion is elaborated on an isothermal tubular reactor system but aims to be used for the linearized model of non isothermal tubular reactors where occur convection, dispersion and reaction phenomena. In this paper the considered reaction is of type $A \to B$ and the system is modeled by the mass balance equation of element A given as second order linear partial differential equation. Existence of solutions for this system in case of constant parameters has been studied in (Le Gorrec *et al.*, 2006) where the authors give the condition to satisfy in order to ensure the existence of a C_0 semigroup. They also propose a parametrization of all the input defining a boundary control system (Le Gorrec *et al.*, 2005). This result is based on the extension of flow and effort variables and the definition of an extended skew-symmetric operator and some coercive closure relations. The existence of solution is then derived from both input matrix condition and coercivity of the closure operator. The previous extension of the operator is not unique and may lead to different input mapping and closure relations.

In this paper, we propose two different parametrizations of the differential operator/closure relation describing the simple isothermal tubular reactor model. In both cases we derive the associated boundary port variables. The Dankwert boundary conditions (Bird , 2002) are then expressed as a linear combination of these boundary port variables and we check the conditions that insure the existence of a C_0 semigroup. We show that existence of solution can be equivalently derived in one case from the coercivity condition of the closure operator and in the other case from the inequality condition on the input matrix mapping. Even if the two initial parametrizations are always possible, the first one can still be applied when the dissipation and the convection depend on the spacial variable while it is not the case with the second one. It will be of particular interest when linearized non linear tubular reactors are considered.

The paper is organized as follows: in section 2 we recall how the differential operator can be parametrized and how from this parametrization one can define a boundary control system. In section 3, we present the model of the tubular reactor with two possible parametrization. For each of them we define the parametrization of the boundary port variables associated with Dankwert conditions. Then we discuss the conditions that has to be checked in order to define a boundary control system. We end in section 4 by conclusion and perspectives.

2. BOUNDARY CONTROL SYSTEM

We consider the class of dissipative boundary control systems:

$$\frac{\partial x}{\partial t}(t,z) = (\mathcal{J} - \mathcal{G}\mathcal{S}\mathcal{G}^*)\mathcal{L}x(t,z) \quad (1)$$
$$u(t) = \mathcal{B}x(t,z),$$
$$y(t) = \mathcal{C}x(t,z),\ x(0,z) = x_0(z)$$

⋆ This contribution has been done within the context of the French National Research Agency sponsored projet HAMECMOP-SYS (ANR-11- BS03-0002) and Labex ACTION (ANR-11-LABX-01-01)

10.1016/j.ifacol.2015.10.230

where $x \in L_2((a,b),\mathbb{R}^n)$ is the state variable. S and $\mathcal{L}$ are positive definite and coercive operators on $L_2((a,b),\mathbb{R}^m)$. Note that S and $\mathcal{L}$ may depend on the spatial variable z. The skew-symmetric differential operator $\mathcal{J}$ is written as:

$$\mathcal{J}x = \sum_i^N P_i \frac{\partial^i x}{\partial z^i} \tag{2}$$

with P_i a real constant matrix in $\mathbb{R}^{(n\times n)}$ satisfying $P_i = (-1)^{i+1}P_i^T$. The differential operator $\mathcal{G}$ and its dual $\mathcal{G}^*$ are defined by :

$$\mathcal{G}x = \sum_i^N G_i \frac{\partial^i x}{\partial z^i}, \mathcal{G}^* x = \sum_i^N (-1)^i G_i^T \frac{\partial^i x}{\partial z^i} \tag{3}$$

with G_i a real constant matrix in $\mathbb{R}^{(m\times n)}$. The operators $\mathcal{B}$ and $\mathcal{C}$ are, respectively, the boundary input and output operators. The system (1) can be rewritten using an extended skew-symmetric operator given hereafter in terms of conjugate port variables, efforts e and flows f, as follows:

$$\begin{pmatrix} f \\ f_r \end{pmatrix} = \underbrace{\begin{pmatrix} \mathcal{J} & \mathcal{G} \\ -\mathcal{G}^* & 0 \end{pmatrix}}_{\mathcal{J}_e} \begin{pmatrix} e \\ e_r \end{pmatrix} \quad , \quad e_r = S f_r \tag{4}$$

with $f = \frac{\partial x}{\partial t}(t,z)$, $e = \mathcal{L}x(t,z)$ and (f_r, e_r) the conjugate port variables associated with the dissipation. The operator $\mathcal{J}_e$ makes explicit the interconnection structure associated with the power continuous energy flows in the system (Duindam et al. (2002)).

Proposition 1. (Le Gorrec *et al.* (2005)) The operator $\mathcal{J}_e$ defined in (4) with (2), and (3) is formally skew-symmetric and can be written as:

$$\mathcal{J}_e \begin{pmatrix} e \\ e_r \end{pmatrix} = \sum_{i=0}^N \overbrace{\begin{bmatrix} P_i & G_i \\ (-1)^{(i+1)} G_i^T & 0 \end{bmatrix}}^{\widetilde{P_i}} \frac{\partial^i}{\partial z^i} \begin{pmatrix} e \\ e_r \end{pmatrix} \tag{5}$$

with $\widetilde{P_i} = (-1)^{i+1}\widetilde{P_i}^T$. Note that $\widetilde{P_N}$ can have a rank deficiency.

In the following, we define the matrices $\widetilde{Q}$, $\widetilde{Q}_1$ and R_{ext} that will be used to define the boundary port variables associated with the extended operator $\mathcal{J}_e$ (see (Le Gorrec *et al.*, 2005; Jacob *et al.*, 2012; Le Gorrec *et al.*, 2006) for more details):

$$\widetilde{Q} = \begin{pmatrix} \widetilde{P}_1 & \widetilde{P}_2 & \widetilde{P}_3 & \cdots & \widetilde{P}_{N-1} & \widetilde{P}_N \\ -\widetilde{P}_2 & -\widetilde{P}_3 & -\widetilde{P}_4 & \cdots & \widetilde{P}_N & 0 \\ \vdots & \ddots & \ddots & \ddots & & \vdots \\ (-1)^{N-1}\widetilde{P}_N & 0 & \cdots & \cdots & & 0 \end{pmatrix} \tag{6}$$

M spanning the column of $\widetilde{Q}$, $\widetilde{Q}_1 = M^T\widetilde{Q}M$ and $M_{\widetilde{Q}} = (M^TM)^{-1}M^T$

$$R_{ext} = \frac{1}{\sqrt{2}} \begin{pmatrix} \widetilde{Q}_1 & -\widetilde{Q}_1 \\ I & I \end{pmatrix} \begin{pmatrix} M_{\widetilde{Q}} & 0 \\ 0 & M_{\widetilde{Q}} \end{pmatrix}, \tag{7}$$

where $I \in \mathcal{R}^{((n+m)N\times(n+m)N}$ is the identity matrix.

Definition 1. The boundary port variables associated with the differential operator $\mathcal{J}_e$ are the vectors $e_{e,\partial}, f_{e,\partial} \in \mathcal{R}^{2nN}$, defined by

$$\begin{pmatrix} f_{e,\partial} \\ e_{e,\partial} \end{pmatrix} = R_{ext} \begin{pmatrix} e_e(b) \\ \vdots \\ \frac{d^{N-1}e_e}{d_z^{N-1}}(b) \\ e_e(a) \\ \vdots \\ \frac{d^{N-1}e_e}{d_z^{N-1}}(a) \end{pmatrix} \tag{8}$$

where $e_e^T = (e, -S\mathcal{G}^*e)$ is the extended vector of effort variables. The following theorem gives the matrix condition that has to be satisfied to ensure existence of solutions and to define a Boundary Control System.

Theorem 2. ((Le Gorrec *et al.*, 2006))Let W be a $(n+m)N \times 2(n+m)N$ matrix. If W has full rank and satisfies the following inequality:

$$W\Sigma W^T \geq 0 \tag{9}$$

where Σ is defined in (7), then the system

$$\frac{\partial x}{\partial t}(t,z) = (\mathcal{J} - \mathcal{G}S\mathcal{G}^*)\mathcal{L}x(t,z) \tag{10}$$

with input

$$u(t) = W \begin{pmatrix} f_{e,\partial} \\ e_{e,\partial} \end{pmatrix} \tag{11}$$

is a boundary control system and the operator $\mathcal{A} = (\mathcal{J} - \mathcal{G}S\mathcal{G}^*)\mathcal{L}$ with domain

$$D(\mathcal{A}) = \Big\{ e \in H^N((a,b);\mathbb{R}^n) \,\Big|\, S\mathcal{G}^*e \in H^N((a,b);\mathbb{R}^n), \begin{pmatrix} f_{f,\partial} \\ f_{e,\partial} \end{pmatrix} \in \ker W \Big\}. \tag{12}$$

generates a contraction semigroup.

Remark 1. To summarize if $\mathcal{A}$ and $\mathcal{G}$ are canonical, the existence of solution is related to the satisfaction of the two following conditions:

(1) S is coercice
(2) $W\Sigma W^T \geq 0$

3. BOUNDARY CONTROL SYSTEM ASSOCIATED WITH THE TUBULAR REACTOR

We consider now a 1D linear tubular reactor of length L, in which occur convection, (axial) dispersion and reaction phenomena. The mass balance equation on species A leads to the following PDE:

$$\frac{\partial \rho_A}{\partial t} = D\frac{\partial^2 \rho_A}{\partial z^2} - v\frac{\partial \rho_A}{\partial z} - k\rho_A \quad , z \in [0, L] \tag{13}$$

where $\rho_A(z,t)$ is the mass concentration of element A, $D > 0$ is the dispersion coefficient, $v > 0$ is the velocity and $k > 0$ the reaction kinetics. Hereafter is proposed two possible ways of writting the model (13) in the general form given in (4). A first one is non canonical since the corresponding differential operator $\mathcal{G}$ depends on the parameters of the system and the second one is obtained by a canonical operator $\mathcal{G}$.

3.1 Case A : Non-canonical formulation

In this case the form (4) of system (13) is obtained using the following parametrization: