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Optimal output-feedback temperature regulation of a catalytic reverse flow reactor PDEs model

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ABSTRACT

In this work, control and estimation problems have been studied for a catalytic reversal flow reactor (CFRR). A stabilizing compensator is developed on the basis of the infinite-dimensional state-space description of the CFRR. Linear–quadratic technique is used to design both an optimal state-feedback controller and an output injection operator. The later is developed based on the duality fact between regulation and estimation. Indeed, the output injection operator is the adjoint of the feedback control operator of the dual process. The developed compensator is tested numerically for the catalytic combustion of lean methane emissions.

1. Introduction

Output-feedback control is a major strategy in system control due to many advantages and it is usually needed when the system states are not available for feedback. Output-feedback regulation is a combination of state-feedback control and state estimation. Indeed, an observer is to be designed to estimate the state of the system and then the feedback is acting one the estimated state. Linear–quadratic control is one of the typical feedback control and is well developed for both lumped parameter systems, i.e systems modeled by ordinary differential equations (ODEs) and distributed parameter systems, i.e systems modeled by partial differential equations (PDEs) or delay systems. The first one is based on finite-dimensional systems theory, however, feedback control problems for PDEs can be solved by using discretization-based finite dimensional representation (see e.g. [1,2]) or infinite-dimensional systems theory (see e.g [3–6]). The latter has a paramount advantage of preserving the distributed feature of the original system. Here, the main objective is to use infinite-dimensional representation to regulate the temperature in a catalytic flow reversal reactor (CFRR).

Catalytic flow reversal reactors (CFRR) are tubular fixed-bed reactors in which the flow direction is reversed periodically. They have a great advantage represented by the fact that the periodic reverse flow creates a heat trap effect allowing auto-thermal operation without external energy supply. This effect is illustrated in Fig. 1. It is a very attractive mode of operation for exothermic reactions since in this case the temperature released from the process can be used and enhanced to keep the process running in the optimal conditions.

CFRRs cover a large classes of chemical processes such as methane combustion, oxidation of sulfur dioxide and oxidation of volatile organic compounds (see [7]). Modeling, design and control of such processes have been the focus of many research works and studies. In [8], a system of PDEs is developed to describe the behavior of a reverse flow reactor. Moreover, an efficient switching strategy is developed to minimize the ammonia leaving the reactor after reversal. On the other hand, some experimental investigations of a pilot reverse flow reactor have been studied in [9]. It has been observed that reverse flow operation maintain high reactor temperatures which helps to achieve high methane conversion. Moreover, the performances of a reverse flow reactor, used for the destruction of lean methane combustion, have been investigated in [10]. In particular, the effect of the extraction on the reactor performances, the effect of the inner type on temperature profiles and reactor stability have been analyzed. In [11], a preliminary study on the control of reversal flow reactor by comparing feedback PID control and model based feedforward control. In [12], model predictive control strategy is implemented in order to reduce the amount of volatile compounds emitted in the atmosphere. The design is based on parabolic partial differential equations model of CFRR. On the other hand, the MPC strategy based on the method of characteristics has been implemented in [13].

Linear–quadratic regulator has been developed for flow reversal reactor in [14] by using dilution and internal electric heating as controls to regulate the hot spot temperature. The optimal control problem has been solved by a discretization-based technique. Indeed, finite-difference discretization is implemented on

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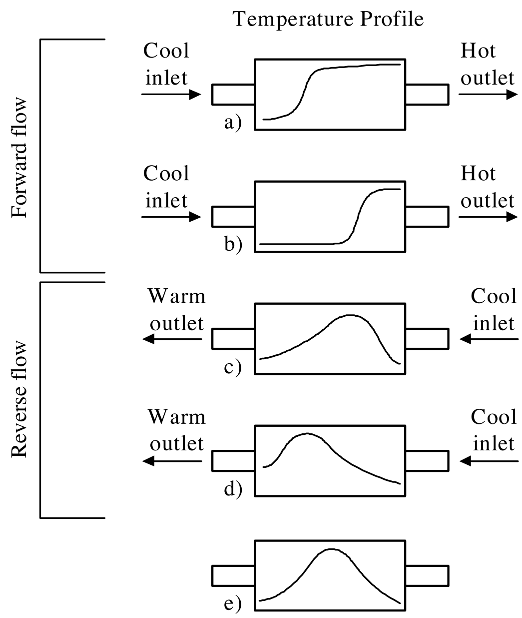

Fig. 1. CFRR heat trap effect.

the linear version of the process to control the temperature at a single location. On the other hand, [15] uses infinite-dimensional system representation to solve the temperature regulation problem associated with the PDEs model of the CFRR. The control of the process is achieved by gas removal based on the manipulation of the fluid velocity along the axis of the reactor at infinite number of points. Such operation is not practical. Moreover, state-feedback control implemented in [15] assumes that the process state is fully accessible which also not feasible from practical point of view. Taking into consideration the above reasons, the objective of this paper is to solve the output-feedback regulation problem for the CFRR by implementing two control strategies. First one is based on gas removal by manipulating the fluid flow velocity at only one location of the reactor, which is more practical than the strategy used in [15] and the second one uses distributed heat exchanger to control the temperature along the reactor. The output-feedback temperature regulation is achieved by using duality feature between the control problem and estimation problem. Indeed, this feature is used to solve the control problem associated with the dual process in order to design a Luenberger observer.

The paper is organized as follows. Section 2 gives a description of the mathematical PDEs model together with its stationary state and its linear version. The optimal control problem is solved in Section 3. Indeed, two types of inputs are investigated, namely distributed input associated with the case of temperature control by using heat exchanger along the reactor and lumped input associated with the case of gas removal at one location of the CFRR. Section 4 investigates the estimation problem to develop a stabilizing compensator. The latter is based on the duality connection between the regulation problem and the estimation problem which suggests that the observer can be developed by solving the linear–quadratic problem for the dual process system. Numerical simulations are performed for the combustion of lean methane to show the performances of the developed compensator.

2. Mathematical model

The dynamics of the catalytic flow reversal reactor is best modeled by PDEs using the material and energy principles. Many different models and configurations have been suggested in the literature to represent the dynamic behavior of CFRR [8,16–20]. Mainly, the difference between most of the models is how heat dissipation is modeled. Here, we consider a pseudo-homogeneous model, which assumes that the solid and fluid temperatures and concentrations are uniform along the reactor [21]. Also, we assume that there are no gradients in the radial direction and finally, we assume plug flow transport phenomena in the axial direction and diffusion is negligible with respect to convection. If Y is the mole fraction of the substance and T is the temperature inside the reactor, then the PDEs model associated with the material and energy principles for the process system with a first order reaction is given by:

$$\begin{cases} \epsilon \dfrac{\partial Y}{\partial t} + \phi v_{in} \dfrac{\partial Y}{\partial \xi} &= -k_0 \exp\left(\dfrac{-E}{R_g T}\right) Y \\ \eta \dfrac{\partial T}{\partial t} + \phi v_{in} \rho \dfrac{\partial T}{\partial \xi} &= (-\Delta H_r) k_0 \exp\left(\dfrac{-E}{R_g T}\right) Y \end{cases} \tag{1}$$

where $t, \xi, \epsilon, v_{in}, \Delta H_r, E$ and R_g are time, space, reactor void fraction, inlet gas flow velocity, heat of reaction, activation energy and universal gas constant, respectively. Also, the parameters k_0, η and ρ are given by

$$k_0 = (1-\epsilon)\mu_{eff} k_\infty, \quad \eta = \rho_s(1-\epsilon)Cp_s \text{ and } \quad \rho = \rho_g Cp_g$$

where μ_{eff}, k_∞, ρ_s, C_{P_s}, ρ_g and C_{P_g} are effectiveness factor, density of solid phase, specific heat of solid phase, density of gas phase and specific heat of gas phase, respectively.

The boundary and initial conditions are given by

$$\begin{aligned} Y(0,t) &= Y_{in} \text{ and } T(0,t) = T_{in} \\ Y(\xi,0) &= Y_0(\xi) \text{ and } T(\xi,0) = T_0(\xi) \end{aligned} \tag{2}$$

Y_{in} and T_{in} are constant and represent the inlet mole fraction and inlet temperature, respectively. Also, Y_0 and T_0 represent the initial mole fraction and the initial temperature profiles, respectively.

Remark 1. To control the temperature in the CFRR, we will adopt as a first scenario gas removal strategy, which remove energy from the system and then the temperature is under control. In this case, the fraction of the inlet gas function ϕ represents the manipulated variable. Here the function ϕ is only time-dependent function since the gas removal is done at one location of the reactor and the input space is $U = \mathbb{R}$. Note that this strategy is implemented by manipulating the fluid flow velocity using a control valve. A second scenario to be adopted here is to use heat exchanger to cool the temperature inside the reactor. In this case, energy balance PDE should include the heat exchange term and can be written as follow

$$\eta \frac{\partial T}{\partial t} + \phi v_{in} \rho \frac{\partial T}{\partial \xi} = (-\Delta H_r) k_0 \exp\left(\frac{-E}{R_g T}\right) Y - h\frac{A}{V}(T - T_c)$$

where h is the heat transfer coefficient and $\frac{A}{V}$ is fluid–solid surface area per unit of volume. Moreover, T_c is the distributed coolant temperature that will play the role of the manipulated variable in the implementation of this second scenario and thus the input space is $U = L^2(0,1)$. Note that in this case we can assume that ϕ is space-varying function but time-independent function.

In order to reformulate the PDEs into an equivalent dimensionless model, let us apply the following classical transformation

$$\tilde{Y} = \frac{Y_{in} - Y}{Y_{in}} \quad \text{and} \quad \tilde{T} = \frac{T - T_{in}}{T_{in}} \tag{3}$$

By using the above transformation, the PDEs model is converted to the following set of PDEs.

$$\begin{cases} \dfrac{\partial \tilde{Y}}{\partial t} = \phi v_1 \dfrac{\partial \tilde{Y}}{\partial \xi} + k_1(1-\tilde{Y})\exp\left(\dfrac{\mu}{1+\tilde{T}}\right) \\ \dfrac{\partial \tilde{T}}{\partial t} = \phi v_2 \dfrac{\partial \tilde{T}}{\partial \xi} + k_2(1-\tilde{Y})\exp\left(\dfrac{\mu}{1+\tilde{T}}\right) \end{cases} \quad (4)$$

where the parameters v_1, v_2, μ, k_1 and k_2 are related to the process parameters through the following equations

$$v_1 = -\frac{v_{in}}{\epsilon}, \quad v_2 = -\frac{v_{in}\rho}{\eta}, \quad \mu = \frac{-E}{R_g T_{in}}$$
$$k_1 = \frac{k_0}{\epsilon}, \qquad k_2 = \frac{(-\Delta H_r)k_1\epsilon}{\eta}\frac{Y_{in}}{T_{in}}$$

In a catalytic reactor, it is typical that the reactant wave propagates with significant larger speed than the heat wave, which implies that the system possess an inherent two-time-scale property, that is, the molar concentration dynamic behavior is much faster than the temperature dynamics. From mathematical point of view, this can be explained by the fact that the constant ϵ is smaller in comparison with η. Moreover, it has been shown in [22] that the fast process is exponentially stable. For these reasons, the dynamics of the mole fraction can be neglected, which reduces the first equation of system (4) to the following ordinary differential equation:

$$\frac{d\tilde{Y}}{d\xi} = -\frac{k_1}{\phi v_1}(1-\tilde{Y})\exp\left(\frac{\mu}{1+\tilde{T}}\right), \quad \tilde{Y}(0) = 0 \quad (5)$$

The above equation is a linear equation relative to $\tilde{Y}$ and it is easy to solve it analytically by setting $\overline{Y} = \tilde{Y} - 1$, which simplifies the equation to the following form

$$\frac{d\overline{Y}}{d\xi} = \frac{k_1}{\phi v_1}\exp\left(\frac{\mu}{1+\tilde{T}}\right)\overline{Y}, \quad \overline{Y}(0) = -1$$

whose solution is explicitly expressed as follows

$$\overline{Y}(\xi) = -\exp\left(\int_0^{\xi}\frac{k_1}{\phi v_1}\exp\left(\frac{\mu}{1+\tilde{T}}\right)d\tilde{\xi}\right)$$

Therefore, the expression of $\tilde{Y}$ is deducted as follows

$$\tilde{Y}(\xi) = 1 - \exp\left(\int_0^{\xi}\frac{k_1}{\phi v_1}\exp\left(\frac{\mu}{1+\tilde{T}}\right)d\tilde{\xi}\right) \quad (6)$$

Replacing the expression of $\tilde{Y}$ in the second equation of system (4) gives the following nonlinear PDE with a single state $\tilde{T}$ and one single input ϕ.

$$\frac{\partial \tilde{T}}{\partial t} = \phi v_2 \frac{\partial \tilde{T}}{\partial z} + k_2 \exp\left(\int_0^{\xi}\frac{k_1}{\phi v_1}\exp\left(\frac{\mu}{1+\tilde{T}}\right)d\tilde{\xi}\right)\exp\left(\frac{\mu}{1+\tilde{T}}\right) \quad (7)$$

In order to solve the output feedback regulation problem, linearization of the above PDE is to be performed. First let us consider $L^2(0, 1)$ the space of square integrable functions on [0, 1] as the state-space. Denote by $\langle \cdot, \cdot \rangle$ the usual inner product in $L^2(0, 1)$, i.e. for any $f, g \in L^2(0, 1)$,

$$\langle f, g\rangle = \int_0^1 f(\xi)g(\xi)d\xi .$$

Let us denote by $\tilde{T}_e$ and ϕ_e the dimensionless profile of the model (7) at the stationary state, which are assumed to be bounded functions on the interval [0, 1] Consider the deviated state and input, respectively:

$$x(t) := x(\cdot, t) = \tilde{T}(\cdot, t) - \tilde{T}_e(\cdot) \in L^2(0, 1) \text{ and } u(t) = \phi(t) - \phi_e \in \mathbb{R} \quad (8)$$

Therefore the linearization of Eq. (7) around its stationary profile leads to the following infinite-dimensional system on $L^2(0, 1)$:

$$\begin{cases} \dot{x}(t) = Ax(t) + Bu(t) \\ x(0) = x_0 \in L^2(0, 1) . \end{cases} \quad (9)$$

where the operator A is defined on its domain:

$$D(A) = \{x : x \text{ is absolutely continuous.,} \; \frac{dx}{d\xi} \in L^2(0, 1) \text{ and } x(\xi = 0) = 0\} \quad (10)$$

by

$$Ax = \alpha\frac{dx}{d\xi} + \beta(\xi)x \qquad \forall x \in D(A) \quad (11)$$

where $\alpha = \phi_e v_2 < 0$ and the function β is given by

$$\beta(\xi) = k_2 \exp\left(\frac{\mu}{1+\tilde{T}_e}\right)\cdot\exp\left(\int_0^{\xi}\frac{k_1}{\phi_e v_1}\exp\left(\frac{\mu}{1+\tilde{T}_e}\right)d\tilde{\xi}\right)\cdot \left[\int_0^{\xi}\frac{k_1}{\phi_e v_1}\left(\frac{-\mu}{(1+\tilde{T}_e)^2}\right)\exp\left(\frac{\mu}{1+\tilde{T}_e}\right)d\tilde{\xi} - \frac{\mu}{(1+\tilde{T}_e)^2}\right] \in L^{\infty}(0, 1)$$

The operator $B \in \mathcal{L}(\mathbb{R}, L^2(0, 1))$ is the linear bounded operator given by

$$B = \gamma(\xi)I, \quad (12)$$

where I is the identity operator and the function γ has the following expression

$$\gamma(\xi) = v_1\frac{d\tilde{T}_e}{d\xi} + k_2\exp\left(\frac{\mu}{1+\tilde{T}_2}\right) \cdot\exp\left(\int_0^{\xi}\frac{k_1}{(\phi_e)^2 v_1}\exp\left(\frac{\mu}{1+\tilde{T}_e}\right)d\tilde{\xi}\right)\cdot \exp\left(\int_0^{\xi}\frac{k_1}{\phi_e v_1}\exp\left(\frac{\mu}{1+\tilde{T}_e}\right)d\tilde{\xi}\right) \in L^{\infty}(0, 1)$$

Remark 2. In the case of heat exchanger, the linearization of the PDE model leads to the same infinite-dimensional system (9) with the following changes to take place. First, α is a distributed bounded negative function given by $\alpha(\xi) = \phi_e(\xi)v_2$ and the input function u and the functions β and γ are changed and given by the following expressions

$$u(t) := u(\cdot, t) = \frac{T_c(\cdot, t) - T_{c,e}}{T_{in}}$$

$$\beta(\xi) = k_2 \exp\left(\frac{\mu}{1+\tilde{T}_e}\right)\cdot\exp\left(\int_0^{\xi}\frac{k_1}{\phi_e v_1}\exp\left(\frac{\mu}{1+\tilde{T}_e}\right)d\tilde{\xi}\right)\cdot \left[\int_0^{\xi}\frac{k_1}{\phi_e v_1}\left(\frac{-\mu}{(1+\tilde{T}_e)^2}\right)\exp\left(\frac{\mu}{1+\tilde{T}_e}\right)d\tilde{\xi} - \frac{\mu}{(1+\tilde{T}_e)^2}\right] - \frac{Ah}{V\eta} \in L^{\infty}(0, 1)$$

$$\gamma = \frac{Ah}{V\eta}$$

In the remaining of this paper, the two scenario are to be distinguished only by the input space. $U = \mathbb{R}$ in case of gas removal and $U = L^2(0, 1)$ in case of heat exchanger.

The following lemma, stating the exponential stability of the unidirectional process, is an immediate consequence of [23, Theorem 2]. Indeed, α and β are bounded functions on [0, 1] and α is negative.

Lemma 1. *Let us consider the operator A defined on its domain by (11). Then the operator A generates an exponentially stable C_0-semigroup e^{At} on $L^2(0,1)$, i.e there are $\kappa > 0$ and $M > 0$ such that*

$$\|e^{At}\| \leq Me^{-\kappa t}$$

Remark 3. Note the exponential stability of the system generator A does not mean necessarily the stability of the catalytic reverse flow reactor. Indeed, the generator A represents the unidirectional process not the reverse flow process as a whole. Also, it is clear that the open-loop reverse flow process (without heat removal or heat exchanger) cannot be guaranteed to be stable due to the fact that trapping the heat in the CFRR will increase the temperature inside the reactor with no guarantee to reach a limited value. The main objective of this work is to develop an algorithm to control, estimate and stabilize the CFRR process.

3. Optimal control

The focus in this section is to design an optimal temperature regulator by solving the linear–quadratic control problem. The design is based on the linearized system described by Eqs. (9)–(12). Here, the output function is given by

$$y(t) = Cx(t) := \int_0^1 c(\xi)x(t,\xi)d\xi = \langle c, x\rangle \tag{13}$$

where the function c is a continuous function on the interval $[0, 1]$. The output function represents the (weighted) average temperature along the reactor and it can be obtained by using a finite number of thermocouples at different locations of the CFRR. The main objective of this paper is to use the output to control the temperature inside the reactor (see Section 4).

The linear–quadratic control problem is: find a square integrable input u_o on $(0,\infty)$ that minimizes the following cost criterion

$$J(x_0, u) = \int_0^\infty \left(|y(t)|^2 + r\langle u(t), u(t)\rangle_U\right) dt \tag{14}$$

where r is a positive function on $[0, 1]$. According to [24], it is known that, the solution of this problem is based on the positive self-adjoint solution $Q_o \in \mathcal{L}(L^2(0,1))$ of the operator Riccati equation (ORE)

$$[A^*Q_o + Q_oA + C^*C - Q_oBr^{-1}B^*Q_o]x = 0, \tag{15}$$

for all $x \in D(A)$, where $Q_o(D(A)) \subset D(A^*)$, where A^* and B^* represent the adjoint operators of A and B, respectively (see [24, Definition A.3.57, p.601]) for the definition of the adjoint operator in general. Moreover, the optimal state-feedback control is given by

$$u_o(t) = -\frac{1}{r}B^*Q_ox(t)$$

The fact that the operator A generates an exponentially stable C_0-semigroup on $L^2(0,1)$ guarantees the existence and uniqueness of a positive self-adjoint solution (see e.g. [24,25]). In order to solve the ORE (15), the adjoint operators of A, B and C are needed.

Lemma 2. *Let A, B and C the operators given by (11), (12) and (13), respectively. Then, the adjoint operator of A is given for all $x \in L^2(0,1)$*

by $$A^*x = -\alpha\frac{dx}{d\xi} + \left(\beta - \frac{d\alpha}{d\xi}\right)x$$

defined on $$D(A^*) = \left\{x : x \text{ absolutely continuous } \frac{dx}{d\xi} \in L^2(0,1) \text{ and } x(1) = 0\right\}$$

The adjoint operator of B is given for all $x \in L^2(0,1)$ by

If $U = \mathbb{R}$, $$B^*x = \langle\gamma, x\rangle = \int_0^1 \gamma(\xi)x(\xi)d\xi$$

If $U = L^2(0,1)$, $B^*x = \gamma(\xi)x(\xi)$

The adjoint of the operator C is given for all $w \in \mathbb{R}$, by

$$C^*w = c(\xi)w$$

Proof. The adjoint of A should satisfy the following equality for all $x \in D(A)$ and $y \in D(A^*)$

$$\langle Ax, y\rangle = \langle x, A^*y\rangle$$

By using integration by parts, one has

$$\langle Ax, y\rangle = \langle\alpha\frac{dx}{d\xi} + \beta x, y\rangle = \int_0^1 \alpha(\xi)\frac{dx}{d\xi}y(\xi)d\xi + \langle x, \beta y\rangle$$
$$= \alpha(\xi)x(\xi)y(\xi)]_0^1 - \int_0^1 x(\xi).\left(\alpha(\xi)\frac{dy}{d\xi} + \frac{d\alpha}{d\xi}y\right)d\xi$$

The fact that $x \in D(A)$ and $y \in D(A^*)$ implies that $\alpha(\xi)x(\xi)y(\xi)]_0^1 = 0$ and therefore

$$\langle Ax, y\rangle = \langle x, -\left(\alpha(\xi)\frac{dy}{d\xi} + \frac{d\alpha}{d\xi}y\right)\rangle + \langle x, \beta y\rangle$$
$$= \langle x, -\alpha\frac{dy}{d\xi} + \left(\beta - \frac{d\alpha}{d\xi}\right)y\rangle$$

which means that the adjoint of the operator A is given for all $x \in D(A^*)$ by

$$A^*x = -\alpha\frac{dx}{d\xi} + \left(\beta - \frac{d\alpha}{d\xi}\right)x.$$

The same process with more easier calculations can be followed to find the adjoints of the operators B and C. □

Since it is known that the operator Riccati equation (15) has a unique positive solution, the main idea here is to check if it admits a solution under the form $Q_o = \omega(\xi)\cdot I$. Indeed, this is an assumption to be validated unless we end up with a contradiction. Under this assumption, it is shown that the ORE (15) can be converted to a differential equation.

Theorem 1. *Assume that $U = L^2(0,1)$. Let us consider the linearized system given by (9). If ω is the unique positive solution of the following differential Riccati equation*

$$\alpha\frac{d\omega}{d\xi}x = \left(2\beta - \frac{d\alpha}{d\xi}\right)\omega x + c\langle c, x\rangle - \frac{\gamma\omega}{r}\langle\gamma, \omega x\rangle = 0, \quad \omega(1) = 0, \tag{16}$$

then the unique positive self-adjoint solution of the ORE (15) is given by $Q_o = \omega(\xi)\cdot I$. Moreover, the optimal state-feedback input is

$$u_o(\xi, t) = -\frac{1}{r}\gamma(\xi)\omega(\xi)x \tag{17}$$

Proof. Assume that the solution of the ORE has the form $Q_o = \omega(\xi)\cdot I$, then based on the expressions of A, B, C and their adjoints operators, Eq. (15) can be written as follows

$$\left[-\alpha\frac{d\cdot}{d\xi} + \left(\beta - \frac{d\alpha}{d\xi}\right)\right]\omega x + \omega\left[\alpha\frac{dx}{d\xi} + \beta x\right]$$
$$+ c\langle c, x\rangle - \frac{\gamma\omega}{r}\langle\gamma, \omega x\rangle = 0$$

$$-\alpha\frac{d(\omega x)}{d\xi} + \beta\omega x - \frac{d\alpha}{d\xi}\omega x + \omega\alpha\frac{dx}{d\xi} + \omega\beta x + c\langle c, x\rangle - \frac{\gamma\omega}{r}\langle\gamma, \omega x\rangle = 0$$

$$-\alpha\frac{d\omega}{d\xi}x-\alpha\omega\frac{dx}{d\xi}+\beta\omega x-\frac{d\alpha}{d\xi}\omega x+\omega\alpha\frac{dx}{d\xi}+\omega\beta x$$
$$+c\langle c,x\rangle-\frac{\gamma\omega}{r}\langle\gamma,\omega x\rangle=0$$

Consequently, the equation becomes

$$-\alpha\frac{d\omega}{d\xi}x+2\beta\omega x-\frac{d\alpha}{d\xi}\omega x+c\langle c,x\rangle-\frac{\gamma\omega}{r}\langle\gamma,\omega x\rangle=0 \quad \square$$

Similar result can be obtained by following the same process in the case of one location input ($U=\mathbb{R}$).

Theorem 2. *Assume that $U=\mathbb{R}$. Let us consider the linearized system given by (9). If ω is the unique positive solution of the following differential Riccati equation*

$$\alpha\frac{d\omega}{d\xi}x=2\beta\omega x+c\langle c,x\rangle-\frac{1}{r}\gamma^2\omega^2x=0,\quad \omega(1)=0, \tag{18}$$

then the unique positive self-adjoint solution of the ORE (15) is given by $Q_o=\omega(\xi)\cdot I$ Moreover, the optimal state-feedback input is

$$u_o(t)=-\frac{1}{r}\langle\gamma,\omega x\rangle \tag{19}$$

4. Compensator design

The optimal state-feedback control needs full information about the temperature in the CFRR, however, this is not feasible. Here, we are interested in designing an observer to estimate the temperature and then develop an output feedback regulator. More precisely, we are interested in developing a Luenberger observer of the form

$$\begin{cases}\dot{\tilde{x}}(t) &= A\tilde{x}(t)+Bu_o(t)+L_o(\tilde{y}(t)-y(t))\\ \tilde{y}(t) &= C\tilde{x}(t)\end{cases} \tag{20}$$

where u_o is the optimal state-feedback control given by Eq. (19) in case $U=\mathbb{R}$ and given by Eq. (17) in case $U=L^2(0,1)$ and L_o is the output injection operator to be found. In order to find L_o, the idea is to solve the linear–quadratic control problem associated with the dual of the linearized CFRR process, which means find the optimal input w_o to minimize the cost criterion

$$\mathcal{J}(z_0,w)=\int_0^\infty\left(\langle v(t),v(t)\rangle_U+\tilde{r}|w(t)|^2\right)dt \tag{21}$$

along the trajectories of the dual linear system

$$\begin{cases}\dot{z}(t) &= A^*z(t)+C^*w(t)\\ v(t) &= B^*z(t)\end{cases} \tag{22}$$

The above problem can be solved throughout the solution of the associated operator Riccati equation

$$[A\Pi_o+\Pi_oA^*+BB^*-\Pi_oC^*\tilde{r}^{-1}C\Pi_o]z=0, \tag{23}$$

for all $z\in D(A^*)$, where $\Pi_o(D(A^*))\subset D(A)$ and the optimal state-feedback control is given by

$$w_o(t)=-\frac{1}{\tilde{r}}C\Pi_oz(t)$$

Moreover, the output injection operator L_o is the adjoint of the optimal state-feedback operator and is given by for all $y\in\mathbb{R}$

$$L_oy=-\frac{1}{\tilde{r}}\Pi_oC^*y(t) \tag{24}$$

Theorem 3. *Let us consider the linearized system given by (9) with input space $U=L^2(0,1)$. Then the unique positive self-adjoint solution of the operator Riccati equation (23) is given by $\Pi_o=\psi(\xi)\cdot I$ where the function ψ is the unique positive solution of the following differential Riccati equation*

$$-\alpha\frac{d\psi}{d\xi}z=\left(2\beta-\frac{d\alpha}{d\xi}\right)\psi z+\gamma^2z-\frac{c\psi}{\tilde{r}}\langle c,\psi z\rangle=0,\quad \psi(0)=0 \tag{25}$$

Moreover, the output injection operator L_o is given for all $y\in\mathbb{R}$

$$L_oy=-\frac{1}{\tilde{r}}\psi(\xi)c(\xi)y \tag{26}$$

Proof. Assume that the solution of the ORE (23) has the form $\Pi_o=\psi(\xi)\cdot I$, whence based on the expressions of A,B,C and their adjoints operators, Eq. (23) can be written as follows

$$\left[\alpha\frac{d\cdot}{d\xi}+\beta\right]\psi z+\psi\left[-\alpha\frac{dz}{d\xi}+\left(\beta-\frac{d\alpha}{d\xi}\right)z\right]+\gamma\langle\gamma,z\rangle$$
$$-\frac{c\psi}{\tilde{r}}\langle c,\psi z\rangle=0$$

$$\alpha\frac{d(\psi z)}{d\xi}+\beta\psi z-\psi\alpha\frac{dz}{d\xi}+\psi\beta z-\psi\frac{d\alpha}{d\xi}z+\gamma\langle\gamma,z\rangle-\frac{c\psi}{\tilde{r}}\langle c,\psi z\rangle=0$$

$$\alpha\frac{d\psi}{d\xi}z+\left(2\beta-\frac{d\alpha}{d\xi}\right)\psi z+\gamma\langle\gamma,z\rangle-\frac{c\psi}{\tilde{r}}\langle c,\psi z\rangle=0 \quad \square$$

Similarly in the case $U=\mathbb{R}$, the following can be proved and stated.

Theorem 4. *Consider the linearized system given by (9) with input space $U=\mathbb{R}$. Then the unique positive self-adjoint solution of the ORE (23) is given by $\Pi_o=\psi(\xi)\cdot I$ where the function ψ is the unique positive solution of the following differential Riccati equation*

$$-\alpha\frac{d\psi}{d\xi}z=2\beta\psi z+\gamma\langle\gamma,z\rangle-\frac{c\psi}{\tilde{r}}\langle c,\psi z\rangle=0,\quad \psi(0)=0 \tag{27}$$

Moreover, the output injection operator L_o is given for all $y\in\mathbb{R}$

$$L_oy=-\frac{1}{\tilde{r}}\psi(\xi)c(\xi)y \tag{28}$$

Finally, we are in a state to write the stabilizing compensator as follows. It is an immediate consequence of the Luenberger observer given by (20) combined with the output injection operator given by (26) in case $U=L^2(0,1)$ or by (28) in case $U=\mathbb{R}$.

Corollary 1. *Let us consider the linearized system given by (9). The stabilizing compensator is given by*

$$\begin{cases}\dfrac{\partial\tilde{x}}{\partial t} &= \alpha\dfrac{\partial\tilde{x}}{\partial\xi}+\beta\tilde{x}-\dfrac{1}{\tilde{r}}\psi c\langle c,\tilde{x}\rangle+\beta u_o+\dfrac{1}{\tilde{r}}\psi(\xi)c(\xi)y\\ u_o(t) &= \begin{cases}-\dfrac{1}{r}\langle\gamma,\omega\tilde{x}(t)\rangle, & \text{If}\quad U=\mathbb{R}\\ -\dfrac{1}{r}\gamma\omega\tilde{x}(t), & \text{If}\quad U=L^2(0,1)\end{cases}\end{cases} \tag{29}$$

where ω is the solution of (16) if $U=L^2(0,1)$ or (18) if $U=\mathbb{R}$ and ψ is the solution of (25) if $U=L^2(0,1)$ or (27) if $U=\mathbb{R}$.

5. Numerical simulations

In order to test the performances of the closed-loop process with the designed compensator, the implementation is based on a CFRR unit for lean methane combustion.

$$CH_4+2O_2\rightarrow CO_2+2H_2O$$

Table 1
Model parameters.

Parameter	Value	Unit
$\overline{M}$	0.029	kg/mole
v_{in}	1	m s^{-1}
k_∞	1.35E5	s^{-1}
R_g	8.314	J mol^{-1} K^{-1}
E	54400	J mol^{-1}
ρ_s	1240	kg l^{-1}
ΔH_r	−802E3	J mol^{-1}
Cp_f	1066	J kg^{-1} K^{-1}
Cp_s	1020	J kg^{-1} K^{-1}
P	101,325	J m^{-3}
μ_{eff}	0.1	

Note that all the results developed earlier are based on the linearized model (9), which represents the unidirectional process. On the other hand, it can be observed that the reverse direction can be also represented by a similar model except that the velocity takes an opposite sign and the boundary condition will be at $\xi = 1$ instead of $\xi = 0$. Indeed, it is represented by the same model (9) with the following main changes in the expression of A and its domain

$$D(A) = \{x : x \text{ is absolutely continuous.}, \ \frac{dx}{d\xi} \in L^2(0,1) \text{ and } x(\xi = 1) = 0\} \quad (30)$$

by

$$Ax = -\alpha \frac{dx}{d\xi} + \beta(\xi)x \qquad \forall x \in D(A) \quad (31)$$

In this case, it is easy to implement the output feedback regulation algorithm in both directions. Moreover, in the case where the input space $U = \mathbb{R}$, it is observed that the reverse direction is generated by the adjoint operator of A and then in this case the implementation is even much easier since the control and the estimation algorithms changes the roles, whenever the flow direction changed and also by taking into consideration changing the roles of the functions γ and β.

To simulate the reverse flow operation of the process, different cycle times have been tested and period of 300 s is chosen, which means full cycle of 600 s is considered here. Model parameters values are given in Table 1 (see [15]). The main objective is to achieve high temperature in the reactor without external heat supply. Two different scenarios can be implemented here. The first scenario is controlling the temperature inside the reactor by heat exchanger, this is associated with distributed input, i.e $U = L^2(0,1)$. The second scenario is controlling the temperature in reactor by removing gas at one location, this is associate with finite-dimensional input, i.e. $U = \mathbb{R}$. This scenario is achieved by manipulating fluid flow velocity at the specific location where gas should be removed. Removal of gas has been shown to be advantageous over cooling by heat exchanger, see [19]. Associated with the gas removed, energy is removed from the system and therefore the temperature is kept under control. The stationary state of the process is given in Fig. 2. It is calculated by solving Eq. (7) at steady state using the inlet values $Y_{in} = 0.03$ and $T_{in} = 298$ K.

In case of distributed input (heat exchanger), the functions ω and ψ are calculated by solving Eqs. (16) and (25), respectively. In order to assess the performance of the compensator, we solved the closed-loop equations under the output feedback control given by compensator (29). Sampling of 100 points are used in order to discretize the PDE model. The resulting deviated response of the closed-loop system together with the input are shown in Fig. 3. It is clear that the state converges to the stationary state. Moreover, the control effort is not aggressive and it can be realized in practice.

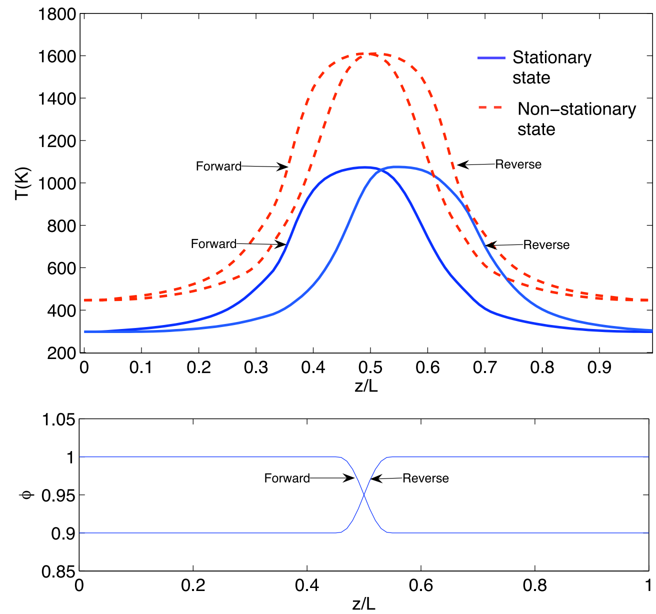

Fig. 2. Temperature at stationary state.

In the case of local gas extraction at one location, the functions ω and ψ are calculated by solving Eqs. (18) and (27), respectively. The resulting deviated response of the closed-loop system together with the input are shown in Fig. 4. Also in this case, the output feedback regulator drives the temperature towards the stationary state but slower than the first case. Indeed, using heat exchanger is equivalent to heat removal at infinite number of locations (not practical), which gives the best achievable control performance compared to heat removal at one location.

6. Conclusion

Temperature regulation and estimation problems have been solved for the catalytic flow reversal reactor. Infinite-dimensional representation is used to describe the PDE model and also to solve output-feedback regulation problem. Two scenarios have been considered here: heat exchanger along the reactor control and gas removal at one location. Control design is done by solving the associated linear–quadratic control problem in infinite-dimensional framework while the observer design is done by using the duality between control and estimation. Output-feedback temperature regulation have been implemented by combining both the controller and the observer. The developed algorithm has been tested numerically on the CFRR for lean methane combustion. Nonlinear closed-loop system analysis is the subject of future investigation. This analysis needs some advanced tools on nonlinear infinite-dimensional systems like the ones developed in [26].

CRediT authorship contribution statement

Ilyasse Aksikas: Conceptualization, Methodology, Formal analysis, Resources, Writing - original draft.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

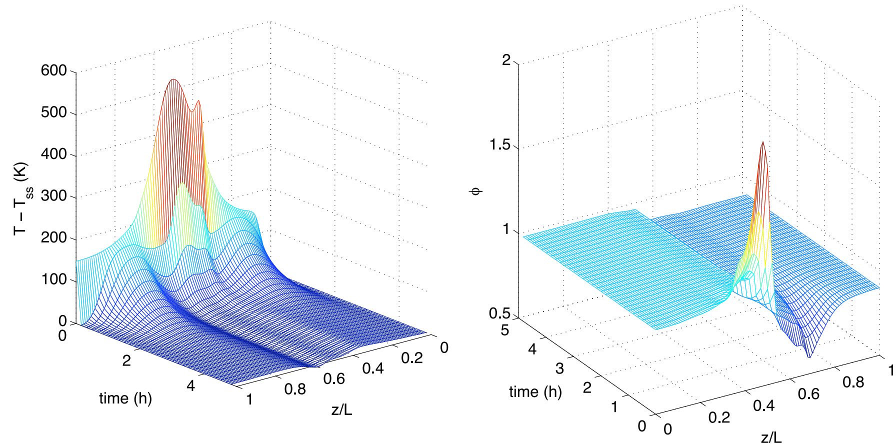

Fig. 3. Left: Closed-loop temperature deviation. Right: Distributed optimal input.

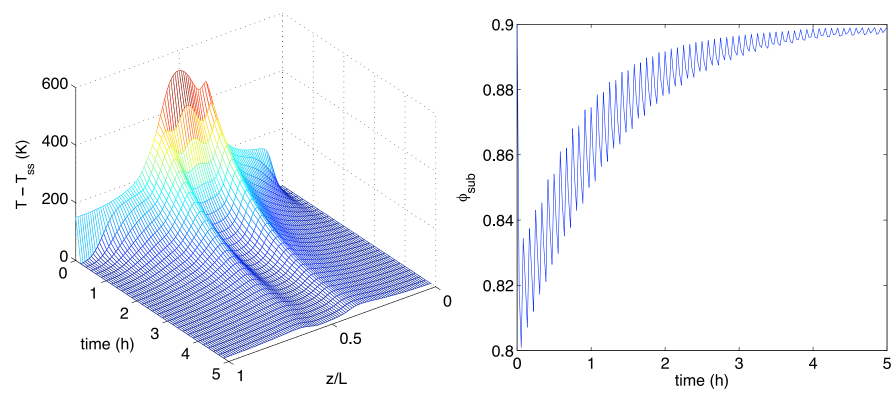

Fig. 4. Left: Closed-loop temperature deviation. Right: Lumped optimal input.

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