Robust PI/PID Controller Design for the Reliable Control of Plug Flow Reactor

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The article presents mathematical description of gas-solid flow reactor and its solution with C++ BzzMath library. This work is illustrating the way of developing the control system of flow reactor with PI/PID controller. Quasi linear regions of output depend on input and disturbance signals were found and several conventional and modern tuning techniques were applied to provide the robustness and performance trade-offs. The system stability was checked for robustness in different regimes (quasi linear and non-linear).

1. Introduction

Nowadays heterogeneous catalysis rules are used in almost industrial processes, especially in the form of heterogeneous gas-solid flow reactors. This equipment has been deeply investigated in chemical engineering history and several modelling strategies have been developed (Manenti et al., 2013). However, these reactors are typically managed by conventional (Proportional-Integral-Derivative, PID) controls and the definition of a smart, effective and robust methodology to tune the control loops may still be a challenge, especially when very exothermic reactions are carried out in these reactors. PID based control systems are those that are commonly employed in the industrial practice because, if they are properly tuned, they can ensure both good performances in servomechanism and regulation problems and the controlled system stability. However, the definition of a proper set of tuning rules, based on a balance between the need for performance and that for stability, is nontrivial. A novel robust PID tuning method, which accounts for both control performance and control stability, has been described elsewhere (Mikhalevich et al., 2015). The goal of the present work is to apply such a technique to tune the PID control system of a catalytic flow reactor (Figure 1). There used notifications: $\rho_i(G)$ is the mass concentration of the i-th component in the reactor, A_{cs} is the reactor vessel cross-sectional area, z is the space position in the axial reactor length, Q is the volumetric flowrate inside the reactor, T is the temperature in the reactor, A_{exc} is the reactor heat exchange area, T_c is the coolant temperature, P is the pressure in the reactor, z_F is the maximum value of z, Q_{IN} is the inlet volumetric flowrate, T_{IN} is the temperature of the reactor feed, P_{IN} is the pressure of the reactor feed, $\rho_i^{(G,IN)}$ is the mass concentration of the i-th component in the reactor feed.
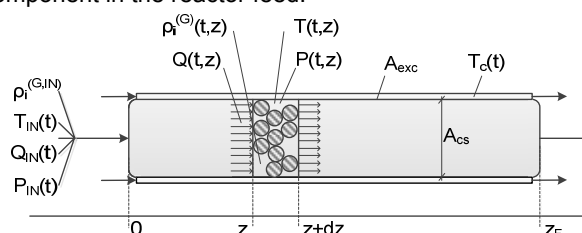

Figure 1: Layout of the catalytic PFR

2. Dynamic model of the plug flow reactor

The plug flow (PFR) reactor, shown in Figure 1, is modeled by means of a first principles approach using the following assumptions to simplify the modeling issues. The reacting mixture is supposed to behave as a perfect gas and its thermodynamic properties (constant pressure and constant volume specific heat, enthalpy of reaction and so on) are considered constant with temperature. Moreover, the gas transport properties (axial dispersion and thermal conductivity, viscosity, global heat transfer coefficient and so on) are assumed to be constant with both temperature and composition. All these assumptions are reasonable for a wide number of different cases. The additional assumptions, introduced for the catalytic phase, include isothermal catalyst and no diffusive limitations inside the catalyst (the efficiency factor equals one). Finally, the reactor temperature is assumed to be controlled with a phase changing fluid, thus there is no variation in the coolant temperature profile with respect to the space.

By exploiting all the reported assumptions and neglecting the gas – catalytic phase gradients, the reactor model is constituted by the component material balances, the energy balance and two additional equations used to predict the pressure losses and the volumetric flow variation. In the end, a pseudo homogeneous model is developed. The material balance for the i-th component is described in Eq(1) while the energy balance can be found in Eq(2):

$$\frac{\partial \rho_i^{(G)}}{\partial t} = -\frac{1}{\varepsilon A_{cs}}\frac{\partial}{\partial z}\left(\rho_i^{(G)}Q\right) + D_i^{eff}\frac{\partial^2 \rho_i^{(G)}}{\partial z^2} + \frac{1-\varepsilon}{\varepsilon}PM_i\sum_{j=1}^{N_R}v_{ij}R_j^{(r)} \tag{1}$$

$$\frac{\partial T}{\partial t} = \frac{1}{\varepsilon\sum_{i=1}^{N_C}\rho_i^{(G)}Cv_i + (1-\varepsilon)\rho_c Cp_c}\left[\begin{array}{l} -\dfrac{Q}{A_{cs}}\sum_{i=1}^{N_C}\rho_i^{(G)}Cp_i\dfrac{\partial T}{\partial z} - (1-\varepsilon)\sum_{j=1}^{N_R}\Delta H_{R_j}R_j^{(r)} + k^{eff}\dfrac{\partial^2 T}{\partial z^2} + \\ +\dfrac{U}{A_{cs}}\dfrac{dA_{exc}}{dz}(T_c - T) - \dfrac{P}{A_{cs}}\sum_{i=1}^{N_C}\dfrac{1}{\rho_i^{(P)}}\dfrac{\partial}{\partial z}\left(\rho_i^{(G)}Q\right) + \\ +P(1-\varepsilon)\sum_{i=1}^{N_C}\dfrac{PM_i}{\rho_i^{(P)}}\sum_{j=1}^{N_R}v_{ij}R_j^{(r)} \end{array}\right] \tag{2}$$

where t is the time, ε is the catalytic bed void fraction, D_i^{eff} is the effective axial dispersion of the i-th component, PM_i is the molecular mass of the i-th component, N_R is the number of chemical reactions, v_{ij} is the stoichiometric coefficient of the i-th component in the j-th reaction, $R_j^{(r)}$ is the rate of the j-th reaction, Cv_i is the i-th component constant volume specific heat inside the reactor, ρ_c is the catalyst intrinsic density, Cp_c is the catalyst constant pressure specific heat, Cp_i is the i-th component constant pressure specific heat inside the reactor, ΔH_{R_j} is the enthalpy of reaction for the j-th reaction, k^{eff} is the effective axial thermal conductivity, U is the global heat transfer coefficient, $\rho_i^{(P)}$ is the density of the i-th pure component.

A Langmuir-Hinshelwood rate equation is chosen (its general functional structure is shown in Eq(3)). Such a rate equation is chosen since the majority of the catalytic reaction kinetics are reported under this formalism in literature:

$$R_j^{(r)} = \frac{k_j^0 e^{Ea_j/RT}\prod_{i=1}^{N_C}P_i^{\gamma_{ji}}}{\left(1 + \sum_{i=1}^{N_C}k_{ji}^{eq,0}e^{Ea_{ji}^{eq}/RT}P_i\right)^{\psi_j}} \tag{3}$$

In Eq. (3), k_j^0 is the pre-exponential factor of the j-th reaction rate constant, Ea_j is the activation energy of the j-th reaction, N_C is the number of components in the reacting mixture, P_i is the partial pressure of the i-th component inside the reactor, γ_{ji} is the reaction order of the i-th component in the j-th reaction, $k_j^{eq,0}$ is the pseudo pre-exponential factor of the equilibrium constant of the i-th component in the j-th reaction, Ea_{ji}^{eq} is the pseudo activation energy of the equilibrium constant of the i-th component in the j-th reaction, RT is the temperature T multiplied by the universal gas constant.

The mathematical expression that can be used to connect the pressure losses to the reactor operating conditions should be derived from the momentum balance. Nevertheless, since the pressure dynamics are much faster than the material/thermal dynamics and of little interest, the dynamic momentum balance can be replaced with the simpler Ergun equation (this equation comes from the momentum balance in steady-state conditions). Ergun equation is stated as follows:

$$\frac{\partial P}{\partial z} = -\frac{1-\varepsilon}{\varepsilon^3} \frac{G}{DP_c \sum_{i=1}^{N_c} \rho_i^{(G)}} \left[1.75G + 150(1-\varepsilon)\left(\frac{\mu_{mix}^{(G)}}{DP_c}\right) \right] \tag{4}$$

where G is the mass flowrate per unit cross-sectional area inside the reactor, DP_c is the catalyst particles diameter, $\mu_{mix}^{(G)}$ is the reacting mixture viscosity.

Finally, a mathematical formula for the evaluation of the volumetric flow is needed. In this model, a simplified expression (Eq(5)), which comes from the perfect gases equation of state, is used.

$$Q = Q_{IN} \left(\frac{T}{T_{IN}}\right)\left(\frac{P_{IN}}{P}\right)\left(\frac{PM_{mix}^{IN}}{PM_{mix}}\right) \tag{5}$$

where PM_{mix} is the molecular mass of the reacting mixture inside the reactor, PM_{mix}^{IN} is the molecular mass of the inlet mixture.

All the model equations have been reported and described but the PDEs require proper initial and boundary conditions to be solved. The initial conditions for Eq. (1-2) consist of the spatial profiles of the state variables at a certain initial time (see Eq(6)) while no initial condition is required for Eq(4). The boundary conditions for Eq. (1-2) have to be imposed both in $z = 0$ and in $z = z_F$ and consist of a set of material/energy balances on the reactor inlet interface (Eq(7)) and a zero gradient condition (Eq(8)), respectively. Once again, Eq(4) is an exception because only the boundary condition in $z = 0$, which comes from a momentum balance on the reactor inlet interface, must be added (Eq(7)).

$$\begin{cases} \rho_i^{(G)}\big|_{t=t_0} - \rho_i^{(G,0)}(z) = 0 \\ T\big|_{t=t_0} - T^0(z) = 0 \end{cases} \tag{6}$$

$$\begin{cases} \left(Q_{IN}\rho_i^{(G,IN)}\right)(t) - \left(Q\rho_i^{(G)}\right)\big|_{z=0} + A_{cs}\varepsilon D_i^{eff} \frac{\partial \rho_i^{(G)}}{\partial z}\bigg|_{z=0} = 0 \\ Q_{IN}(t)\left(T_{IN}(t) - T\big|_{z=0}\right)\sum_{i=1}^{N_c} \rho_i^{(G,IN)}(t)Cp_i^{IN} + A_{cs}k^{eff}\frac{\partial T}{\partial z}\bigg|_{z=0} = 0 \\ P\big|_{z=0} - P_{IN}(t) = 0 \end{cases} \tag{7}$$

$$\begin{cases} \dfrac{\partial \rho_i^{(G)}}{\partial z}\bigg|_{z=z_F} = 0 \\ \dfrac{\partial T}{\partial z}\bigg|_{z=z_F} = 0 \end{cases} \tag{8}$$

In Eq(6-8), t_0 is the initial value of t, $\rho_i^{(G,0)}$ is the mass concentration of the i-th component inside the reactor at $t = t_0$, T^0 is temperature inside the reactor at $t = t_0$, Cp_i^{IN} is the i-th component constant pressure specific heat in the reactor feed.

All the equations and the proper initial/boundary conditions belonging to the reactor model have been shown but these equations must be solved with a suitable numerical method, thus some information on the model solution approach must be added. Here, the finite difference method, based on backward derivatives approximation, is employed. In detail, all the reported equations are discretized in space in order to reduce the PDAE system to an initial value DAE system. Then, the DAE system is solved by the BzzMath DAE integrator (Buzzi-Ferraris and Manenti, 2012), which is based on improved Gear multi-value methods. In order to ensure an elevated efficiency in the discretized PFR model solution, it is mandatory to exploit the system Jacobian structure (Figure 2). The BzzMath DAE integrator can be provided with the Jacobian matrix sparsity pattern, thus it is suitable for this application.
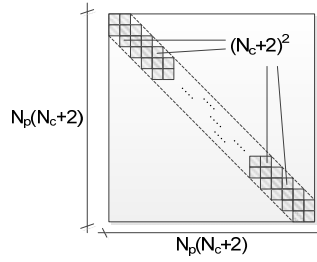
Figure 2: Sparsity pattern of the Jacobian of the discretized PFR reactor model

3. Development and tuning of the PFR control system

The proportional-integral (PI) and proportional-integral-derivative (PID) controllers are widely used in industry (Visioli, 2012). This type of control is the most popular because a wide class of industrial processes can be in control of it. According to this remarks, the authors have decided to use the control system presented in Figure 3.

Nowadays there are a lot of techniques (Aström and Hägglund, 2005) for the optimal calculation of the parameters of PI/PID controllers and ones modifications (Shamsuzzoha, Al-Mutairi, 2011). Each of them has advantages and disadvantages. Therefore, the authors have chosen several modern and conventional PI/PID tuning methods and have applied them to the proposed control system in and compare their performance.

An identification procedure must be completed before PID tuning can be obtained. For this purpose the step response of the PFR model is computed and, subsequently, used to generate a simplified linearized model, based on a transfer function representation. Note that the identification is performed by using T_e as the only manipulated variable and T_{out} as the only controlled variable of the PFR. The transfer function resulting from the identification is presented in Eq(9).
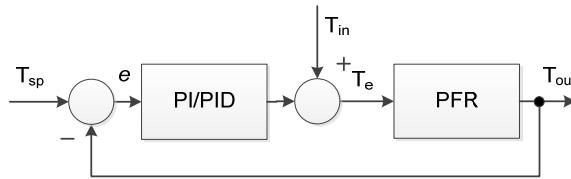

Figure 3: PFR control system where T_{sp} is the PFR hot spot temperature set-point, T_{in} is the temperature of the PFR inlet flowrate, T_{out} is the PFR hot spot temperature

$$PFR(s) = \frac{0.477}{89s+1}$$

(9)

The transfer function of PFR is true for linear bounds shown on Figure 4. These bounds required for the functionality of the control system must be coupled with the physical constraints. It must be ensured that T_e < 525 K and T_{in} ∈ [425;485] K (according to the technical requirement). After combining theoretical and practical bounds, the final allowed intervals for T_e and T_{in} are: T_e ∈ [395;525] and T_{in} ∈ [450;485].

Notice that the PI/PID controller in the proposed control system must consider the saturation for the control signal according to the T_e bounds, described above. As an alternative, we may suppose that our reactor is an interval system and, subsequently, tune the PI/PID controller as for an interval system (i.e., each parameter of the transfer function is not constant). In this latter option, we need to check the behavior of the control system in the case of nonlinear response of the target process.
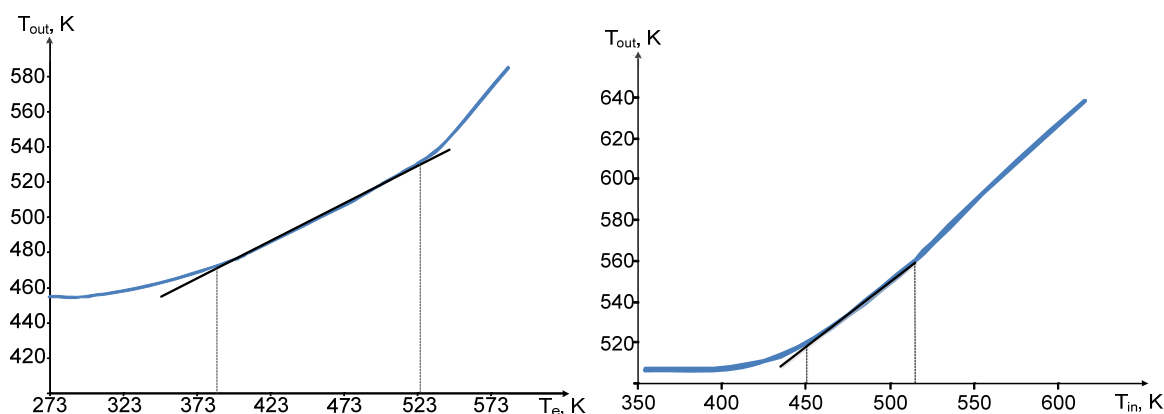
Figure 4: Identification of the quasi-linear operation regions

In order to tune the PI/PID controller in proposed control system, the authors have used several methods. Magnitude Optimum (MO) (Aström and Hägglund, 2005) provides the maximum bandwidth of system. Mikhalevich et. al. (Mikhalevich et al., 2015) provides minimal overshoot for desired phase margin and crossover frequency. Good Gain Method (Haugen, 2012) is an alternative of Ziegler-Nichols (Ziegler and Nichols, 1942) that provides better stability robustness with Ziegler-Nichols method.. Also, several control quality and robustness indexes have been evaluated: maximum sensitivity (M_s), phase margin (φ_m), and settling time (t_s).

The results of the servomechanism and disturbance attenuation, in the region where the reactor response is almost linear, are presented in Figure 5. The control systems tuned by means of the Good gain method is not shown because the PFR becomes unstable. The control system performance measures and robustness indices are shown in Table 1.

According to Figure 4, the PFR reactor is a nonlinear system. Therefore, we need to check the performance of the control system, tuned with different methods, also based on a servomechanism problem performed in the region where the reactor response is nonlinear. The results of this servomechanism problem are presented in Figure 6. According to Figures 5, Figure 6 and Table 1, the most appropriate control system for a PFR appears to be a PID, tuned by the Mikhalevich et. al. method. It provides minimum overshoot and settling time along with reasonably large robust indices. The proposed PID controller also allows both to exclude the saturation block from the control system and to control the reactor over the entire range of feasible operation.

Table 1. Control system performance and robustness when different tuning methods are employed

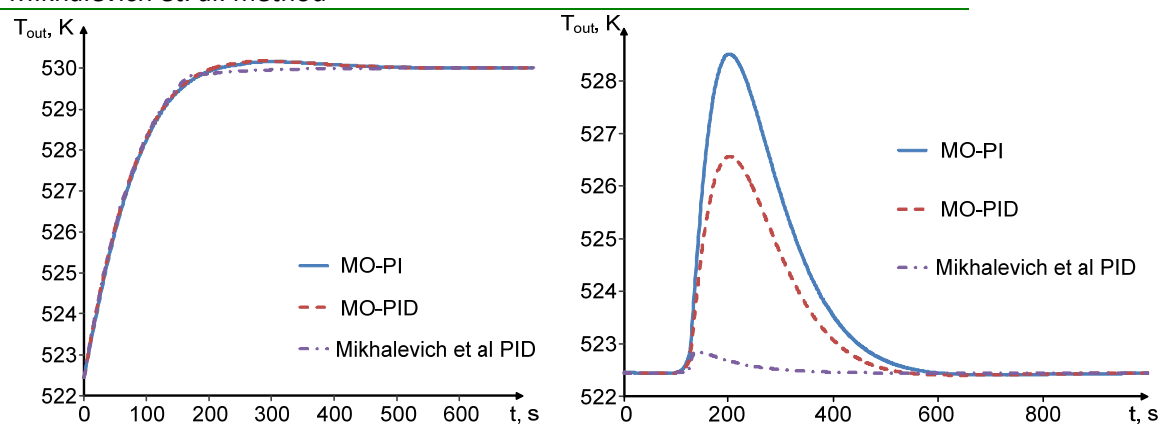| Method	Settling time, s	Maximum sensitivity	phase margin, °
MO-PI	179	1	78.49
MO-PID	175	0.67	105.3
Mikhalevich et. al. method	165	0.81	104

Figure 5: PFR transient in a servomechanism and disturbance attenuation problem (the reactor response is quasi-linear)
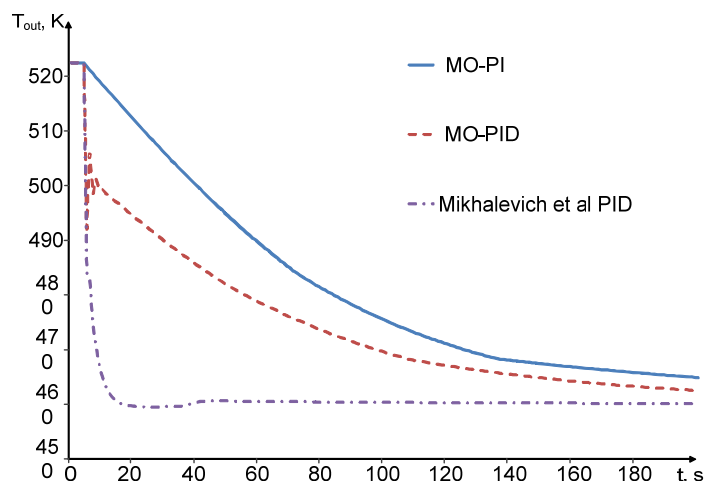
Figure 6: PFR transient in a servomechanism problem (the reactor response is nonlinear)

4. Conclusions

This paper has outlined a mathematical model of a catalytic flow reactor, made of partial differential equations, algebraic equations and boundary conditions. Then, the PFR dynamic behavior has been approximated with a first order transfer function (FOTF) without delay time and the regions of linear dynamic response have been identified as a function of the manipulated variable and the external perturbation. Despite the widespread belief that the best controller for chemical plants is a PI, both PI and PID controllers have been tested. Their tuning procedures have been addressed with several methods. The performances of the PI/PID controllers, all tuned with different strategies, have been compared on several servomechanism and disturbance attenuation problems in the region where the PFR exhibits both a quasi-linear and a nonlinear behavior. It results that PID appears superior to PI, in contrast to the standard beliefs, and the Mikhalevich et al. (2015) method ensures the best performances. Finally, a modern PID tuning method has been used to develop a reliable and efficient control system for PFR reactors.

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