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Advanced Control Algorithm for a Chemical Polymerization Process

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Abstract: This study deals with the study of simulated implementation of non-linear control algorithm for temperature stabilization of a CSTR reactor to maintain favorable ethylene conversion and butene1 yield conditions. The simulation results revealed the capability of all the proposed control algorithms to stabilize such a reactor with some differences in their performance.

Key words: Ethylene dimerization, temperature stabilization, fuzzy logic control

INTRODUCTION

FLC is a nonlinear controller and can adapt itself to changing situations; it can outperform conventional PI controllers for unstable dynamics and nonlinear systems. In contrast to model-based controllers, FLC is known as a knowledge-based controller that does not require a mathematical model of the process at any stage of the controller design and implementation. In many cases, the phenomenological model of the control process may not exist or may be too expensive in terms of computer processing power and memory and a system based on rules of human knowledge may be more effective.

Reactor model: The dimerization reactor (Assala *et al*., 1997) considered in this study is assumed to be a liquid phase perfectly mixed reactor. Schematic of the process is depicted in Fig. 1. The liquid is homogenized by a high re-circulation rate around the reactor through a heat exchange used to remove the high exothermic heat of reaction. The model uses the Homo and Co-polymerization mechanisms suggested by Gauthier (Assala *et al*., 1997).

Based on the above assumptions and the assumed reaction kinetics, the resulted dynamic model (Alhumaizi, 2000) of the dimerization process is as follows:

$$V\frac{dC_4}{dt} = -Q\beta C_4 - V \left[(-b_2C_2 + a_4C_4 + b_4C_4)K_2 + a_4C_4K + b_4C_4K_4\right] \quad (1)$$

$$V\frac{dC_2}{dt} = FC_{2f} - Q\beta C_2 - V \left[a_2C_2(K + K_2 + K_4) + b_2C_2(K_2 + K_4 + K_6)\right] \quad (2)$$

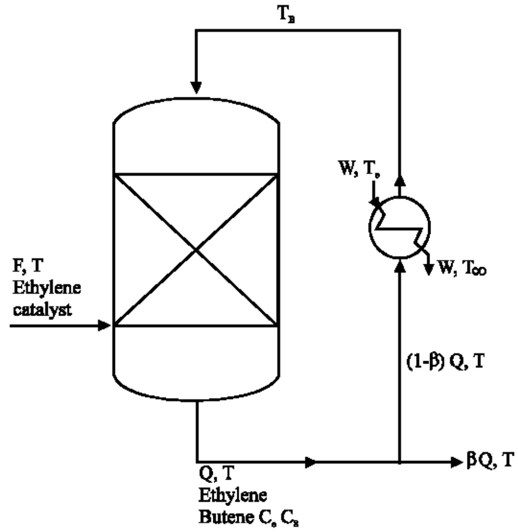

Fig 1: Schematic of the dimerization reaction process

$$V\frac{dK}{dt} = FK_f - Q\beta K - V \begin{bmatrix}(a_2C_2 + a_4C_4)K + b_2C_2(K_2 + K_4 + K_6) \\ +b_4C_4(K_2 + K_4)\end{bmatrix} \quad (3)$$

$$V_\rho C_p\frac{dT}{dt} = F_{\rho f}C_{pf}(T_f - T_r) + Q(1-\beta)\rho C_p(T_R - T_r) - Q_\rho C_p(T - T_R) + V(r_2(-\Delta H_1) + r_4(-\Delta H_2)) \quad (4)$$

$$V_e pC_p\frac{dT_R}{dt} = Q(1 = \beta)pC_p(T - T_R) - UA(T_{Rav} - T_{cav}) \quad (5)$$

$$V\frac{dK_2}{dt} = -Q\beta K_2 + V \left[a_2C_2K - (a_2C_2 + a_4C_4 + b_2C_2 + b_4C_4)K_2\right] \quad (6)$$

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$$V\frac{dK_4}{dt} = -Q\beta K_4 + V \left[a_2C_2K_2 - (a_2C_2 + b_2C_2 + b_4C_4)K_4 + a_4C_4K\right] \quad (7)$$

$$V\frac{dK_6}{dt} = -Q\beta K_6 + V\left[(a_2C_2K_4 - b_2C_2K_6 + a_4C_4K_2)\right] \quad (8)$$

The dynamic of the outlet temperature of the coolant fluid is not included and alternatively it is obtained by solving the steady-state equation:

$$WCp_w(T_{co} - T_c) + U_hA_c(T_{Rav} - T_{cav}) \quad (9)$$

In this case, W (Coolant flow rate) and F (Gases feed flow rate) are used as forcing inputs. The kinetic parameters are used in this study are based on the rate constants. The original model of the dimerization process contains two additional states. The two states, which represent the hexane and octane concentrations, are not included in this paper for simplicity. This assumption is valid since the above eight states are independent of the omitted ones.

Open-loop analysis: Our previous open-loop bifurcation analysis, revealed the existence of a trade-off between conversion and selectivity (yield), which is clear in Fig 2. It can be seen that as the feed flow rate F increases, the conversion increases while the yield decreases and vise verse. For this reason it is recommended to operate the plant around a favorable operating point that corresponds to F = 4×10-3 m^3/s, which corresponds to 95.7% conversion and 69.6% yield. This point also corresonds to a practical temperature operation, which has to be around the heavy mixture bubble point of 67°C. Nevertheless, as the open-loop response shown in Fig. 3 indicates, the desired operating point is unstable. The stable regions for this process are economically unacceptable. For example, as shown in Fig. 2 a stable region exists at high throughput. Another stable region is located at very low F, which corresponds to a high selectivity but low conversion and production rate. This region is not shown in the Fig. 3. Therefore, there is a potential for utilizing a good control design to stabilize the reactor around the desired open-loop unstable point.

Control objective: The main control objective of such a process is the stabilization (Assala *et al.*, 1997) of the reactor temperature. This is essential to secure safe plant operation and to deliver a good quality product. It is also desirable to maintain optimal operation of high ethylene conversion and desired butene-1 yield in the face of plant upsets. In practice, the coolant feed temperature, Tc, is one possible source of disturbances to the process, which may cause thermal runaway due to temperature instability and consequently loss of conversion and/or yield. The upset in Tc is chosen for demonstration purposes and is considered to simulate an unknown unmeasured disturbance that creates a temperature excursion situation. For this reason, the closed-loop simulations in this paper focus on temperature stabilization and maintaining desired yield in the face of upsets in Tc. In this case, the controlled variable would be the reactor Temperature, (T) and the butene concentration at the outlet stream, (C4). In due course, the suitable Manipulated Variables (MV) are the coolant flow rate, W and the feed flow rate F. Single-Input Single-Output (SISO), Multi-Input Single Output (MISO) and MIMO control schemes will be examined for this control problem. For the SISO case, the controlled

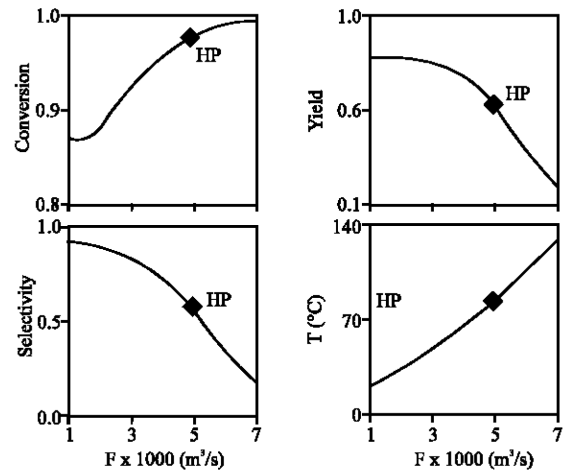

Fig. 2: Steady state bifurcation diagram

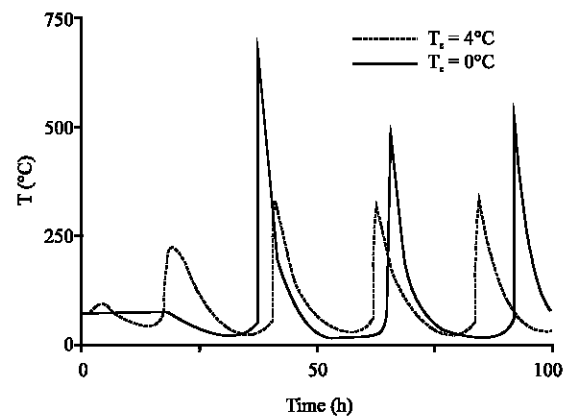

Fig. 3: Open loop simulation of the reactor temperature for two values of T_c

variable is the reactor temperature and the manipulated variable is the coolant flow rate. The MIMO scheme is carried out in a decentralized form where T is regulated via W and C4 via F. The selection of these particular manipulated variables includes detailed analysis for designing the control structure of the dimerization reactor. In the simulation section, a sampling rate of 0.1 h will be used, which is more realistic for practical applications.

Fuzzy logic control algorithm: The basic FLC loop (Alvarez, 1996) is shown in Fig. 4. It consists of 3 major sequential steps, namely Fuzzification, Inference engine and Defuzzification. In the following subsections, the development and design of each step is discussed in detail. Hereafter, by input we mean controller input, i.e., error and/or error velocity signal and by output we mean the controller output, i.e., manipulated variable.

Fuzzification: The input signal of the controller, which is a real-value variable also known as crisp value, is fed to the fuzzifier. In the fuzzifier, the crisp value is converted as a member of a finite number of fuzzy sets. Therefore, the process of fuzzification is simply mapping, i.e., checking the value of the input signal (member) against each fuzzy set to determine its degree of membership. The fuzzy set is usually represented as a membership function as shown in Fig. 5. The membership function can have any symmetrical geometric shape and is graded between 0 and 1. The fuzzy sets in Fig. 5 are identified by linguistic variables such as Large Positive (LP), Small Positive (SP), Zero (ZE), Small Negative (SN), Large Negative (LN) and they are labeled as 1, 2, 3, 4 and μ5, respectively. Usually, finite number of overlapping membership functions (fuzzy sets) (Bernard, 1988) can be used to span the possible range of the process variable. The overall span is known as the universe of discourse.

Common difficulties exist in this step. The selection of the shape and number of the membership functions, the location of their center. Moreover, the common FLC design involves at least three different groups of fuzzy sets, each of which corresponds, to a different process variable. For example one group is used for the error signal, e, another for the velocity of error signal, e and another for the controller's output (manipulated variable), u. The latter is used in the defuzzification step. In this paper we try to overcome the above problems. First we use only one group of fuzzy sets for all the three process variables. To achieve this, the universe of discourse is unified so that it spans the interval [-1, +1]. In this case, the value of each process variable should be scaled properly to fit the specific interval. Secondly, Gaussian and sigmoidal shapes are considered for the membership

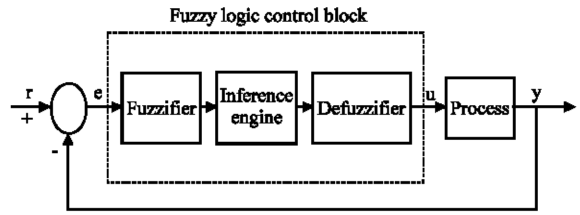

Fig. 4 : Block diagram of the FLC algorithm

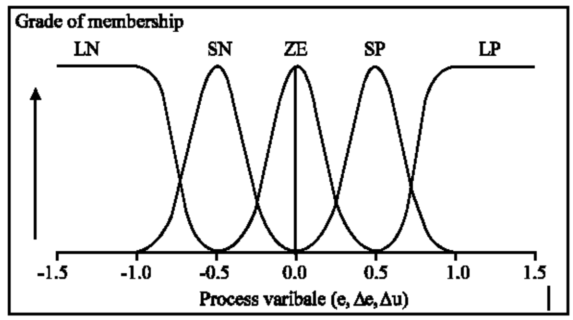

Fig. 5: Gaussian fuzzy set used in this study

functions. Gaussian shape is selected because it is a continuous function and can be easily expressed by an analytical formula. Continuity of the Gaussian functions produces smoother control output. Usually to symmetrically span the input domain, odd number of fuzzy sets should be designed. Increasing the numbers of the fuzzy sets creates smoother output. However, this will be at the expense of increasing the number of control rules leading to more complicated design procedure and tuning. Therefore, five such functions are used here as shown in Fig. 5, which found, with the aid of Gaussian functions, sufficient to provide smooth output at reasonable number of fuzzy rules.

In this research two variables are fuzzified, which are the error (e) and the error velocity (.e). Therefore, in this controller phase, the membership degree of a specific input value, i.e., e or e, over all fuzzy sets can be determined directly from Fig. 5.

Inference engine: Inference engine is the heart of the FLC algorithm where the control action is formulated. In this study, we choose to design the rule base according to desired response of the process because it the most intuitive for many control practitioners.

At this phase of the controller algorithm, given a value for the input signal, the degree of fulfillment of each rule in the rule base set is determined. The degree of fulfillment of the rule base is known as the conclusion or the result of the rule base. The process in which these conclusions are calculated is known as inference. Due to overlapping membership functions, some of the rule conclusions may have a zero value and some a non-zero value.

Membership function for the output with a non-zero degree of fulfillment is considered fired. In standard FLC algorithms, the fired functions are clipped or scaled and then copied to a temporary template. All fired sets are then combined using superimposing technique. The combined set is known as the inferred controller output. Figure 6 shows an example of three combined active fuzzy sets.

Defuzzification: In this step, the combined output fuzzy sets are then converted into a single crisp value. The calculated crisp value is the numerical value for the manipulated variable. In standard FLC applications, the combined set is a new geometric shape; say µout (Fig. 6). Hence, finding a weighted average is similar to determining the geometric center. One way is by calculating the center of area. The discretized form of COA can be written as:

$$\Delta u = \frac{\sum_{j=1}^{n_R}\sum_{i=1}^{n_f}\mu_{j,i}\,\delta_i\,A_{j,i}}{\sum_{j=1}^{n_R}\sum_{i=1}^{n_f}\mu_{j,i}A_{j,i}} \quad (10)$$

Where nf is the number of output membership functions and equals 5 in this study, nR is the number of rules and equals 25 in this study, which is the maximum possible number to cover all eventualities created by the 5 output membership functions. δi is value for the location of the center of µi. The value of äi is pre-calculated and fixed as shown in Fig. 5. A is nR x nf pre-calculated matrix, which identifies which membership function is included in each rule. For example, row 1 of matrix A, which is assigned for Rule 1, contains 1 at the first column and zeros elsewhere. The same logic is carried out over the remaining rows.

It should be emphasized that the control output, u computed by Eq. 10 is taken in the velocity form. Velocity form is more suitable for non-linear systems. In non-linear systems, the new equilibrium value for u, denoted as uss, that brings the output to the desired steady state value may not be known beforehand. Thus, it is difficult to locate uss in the universe of discourse as the center for the ZE membership function. However, when u is used, zero value will always be the equilibrium point around which ZE can be built.

Tuning method: Tuning a fuzzy linguistic controller to changing process and environment dynamics can be accomplished in several different ways:

- Adjusting the membership functions.

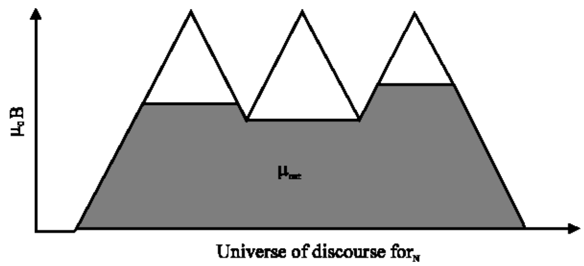

Fig. 6: Example of clipped output membership function

- Changing the finite set of values describing the universe of discourse.
- Reformulating the finite set of control rules in the knowledge base (inference engine).

However, these procedures are cumbersome. In addition, there are no clear guidelines on how these procedures affect the closed-loop response. In this paper, we adopt a simpler method. The scaling factors for the input and output signals are used as the tuning parameters. As will be seen in the examples, these factors have direct and clear effect on the closed-loop response. These factors are used to scale the process variables so that they fit the universe of discourse domain used in Fig. 5. Specifically, the scaling factors for the error, error velocity and output velocity are se = a/sp, sde = b/sp and sdu = c.um, respectively. For servo control problems, sp is the difference between the set point and the initial steady state value for the controlled variable. For regulatory control problem, p is the set point value um is the difference between the maximum and minimum allowable values for the manipulated variable. Therefore, a, b and c are the tuning parameters. Changing the value of a, b, or c is equivalent to stretching or expanding the universe of discourse of the fuzzy sets shown in Fig. 5. Conceptually, this is similar to the first two tuning guidelines mentioned above.

FLC algorithm: The following steps explain the FLC control (Bernard, 1988) algorithm used in this study.
Set a = b = c = 1. At any sampling time, k do:

Step 1: Scale the error and the error velocity signals (e (k), e (k)) via multiplying them with se and sde.
Step 2: Compute the degree of membership of e(k) and e(k) to the five membership functions shown in Fig. 5.
Step 3: Calculate the conclusions of the Rule base.
Step 4: Calculate the control action using equation 10. Scale the computed value by multiplying with sdu.
Step 5: Implement the control action, set k=k+1 and go back to step 1.

If the control performance is poor, adjust the value of a, b, or c. We have found that increasing the value of a increases the speed of response and eliminates offset. Increasing the value of c penalizes the manipulated variable moves, thus introduces stabilizing effect.

Closed-loop simulations fuzzy logic controller: The above SISO, MISO and MIMO control problems are re-tested using the FLC algorithm (Garrido *et al*., 1997). Regarding the SISO case, Fig. 7 demonstrates the closed loop response to two step changes in Tc of +4 and +6°C, respectively. For both cases, a = 1, b = 10 and c = 105 are used. As the figure illustrates, a perfect disturbance rejection without offset is obtained for the first case, i.e., Tc = +4°C. For the larger disturbance case, i.e., Tc = +6 °C, poor performance, which seems worse than that for the PI algorithm, is obtained. The poor temperature control is associated with a loss in the yield, which is not shown in Fig. 7 for simplicity. The SISO FLC performance can be made less aggressive through tuning. However, the closed-loop response will eventually oscillate due to input saturation. The SISO PI response also oscillates if aggressive values for the tuning parameters are used or if longer simulation time is used. Anyhow, further improvement in the FLC performance is not possible in this case because the loss in performance is due to input constraints.

Building upon the poor performance faced in the SISO case at large upset in the inlet cooler temperature, a MIMO FLC scheme is examined. In this case, a decentralized control system similar to that used in the PI algorithm is also used here. The result of the closed loop response is shown in Fig. 7 by the solid lines.

For the first loop, a = 1, b = 100 and c = 105 are used, while a = 1, b = 3×second loop. Tuning is found to be a cumbersome task due to the strong cross interaction. Nevertheless, the obtained closed loop response is reasonable as perfect control of T and minor offset in C4 (-67 mole m^{-3}) are observed. Small reduction in the feed flow rate was necessary to reduce offset in the yield, but was not good enough. Further tuning was found not helpful. The FLC tuning parameters are the same as in the MIMO case except that c for the second loop is re-adjusted to 1×10-4. The only reported advantage of the FLC is that its resulted performance for the MISO case outperforms that obtained by the PI algorithm. However, the MISO FLC is superior to the MIMO FLC in the sense of less offset in the yield response. This situation is attributed to the strong cross-lop interaction. In the MIMO case, tuning the second control loop to reduce offset in the yield would require less fresh feed flow. Alteration of the fresh feed flow introduces disturbance to the first control loop leading to temperature runaway and consequently unstable process behavior. Moreover,

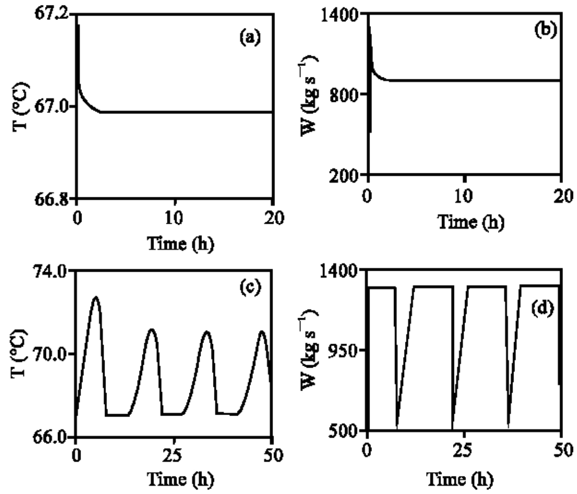

Fig. 7: Closed loop rsponse to step changes in T_c using SISO FLC algorithm (a,b): Δt_c = +4°C, (c,d): Δt_c = +6°C

it is found that tuning the FLC parameters for the MIMO case is as difficult as that for the MIMO PI algorithm.

CONCLUSION

Our previous closed loop analysis using a first-principle model for the ethylene to butene-1 dimerization reactor revealed the necessity for a better control design. For this purpose nonlinear control strategies such as fuzzy logic, was tested for possible stabilization of such a reactor. Application of SISO FLC algorithms revealed the ability to stabilize the reactor at a low upset in the coolant temperature. At high upsets, saturation of the coolant flow rate occurs degrading the controller performance. This founding is in agreement with that obtained previously. The limitation of the SISO scheme is not related to the control algorithm neither to controller tuning, but rather to the controllability of the process.

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