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THERMODYNAMIC PREDICTIVE FUNCTIONAL CONTROL APPLIED TO CSTR WITH JACKET SYSTEM

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Abstract: The objective is to control the internal temperature of a continuous stirred tank reactor (CSTR) with jacket and analyze the potentiality that offers manipulating the thermodynamic conditions of the coolant flow. In this paper four predictive functional control (PFC) strategies are analyzed, two of them are conventionally structured by manipulating flow in one case and temperature of the jacket coolant in the other. The other two manipulate the enthalpic conditions of the coolant in a cascade form by setting flow and temperature optimally. The servo and regulator problem are analyzed including an statistical economic studio for defining the best control structure. *Copyright © 2002 IFAC*

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1. INTRODUCTION

The most reaction system in the chemical industries are exothermic so the control system must ensure that the reaction heat is removed from the reactor to maintain a steady state. Failure to remove the heat of reaction would lead to an accumulation of heat within the system and rise the temperature. Therefore temperature is a good controlled variable since it is easy to measure and it has close thermodynamic relation to heat (Luyben et al., 1999). Accounting with these issues four predictive control strategies are analyzed in order to handle efficiently the thermodynamic conditions on continuous stirred tank reactors (CSTR) with jacket.

The use of PFC technology is evaluated for driving the system to an optimal operation and economic point. The PFC technique is the third generation of a family of Model Algorithmic Control (MAC), developed by Richalet and coworkers during the last decades (see Richalet, 1993). It resides on represent the plant with a linear impulse response model, generate the control algorithm for one or more coincidence points with the reference trajectory, solve it and apply the calculated input action. The later can be constrained on its maximum and minimum values and its rate of variation.

2. MATHEMATICAL CALCULATIONS FOR PFC DESIGN

For PFC the structure of the model and its parameters are estimated by any identification algorithm available which exploits the data collected during specific step test experiments. The model is used to predict the future process output and to compute the control action in order to satisfy a given target (C) for the process variable (PV).

PFC basically consists of the same elements as can be seen in Fig. 1: the dynamic model; a reference

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trajectory $y_r(n)$ which describes the smooth transition of the target variable from its current value to the future set point profile within a prediction horizon that corresponds to the end of the coincidence horizon. This trajectory can be interpreted as the desired behavior of the closed loop system. The future error between the reference trajectory and the predicted output over the coincidence horizon [H_1, H_2] is estimated. For the case study analyzed here only one coincidence point and a constant set point C is assumed. It will be developed the control law for first order with time delay on both plant (Gmi) and perturbation model (Gdi).

$$Gmi(s) = Gmi.\frac{1}{1+\tau_{mi}.s} \tag{1}$$

$$Gdi(s) = Gdi.\frac{1}{1+\tau_{di}.s} \tag{2}$$

Applying the Z-transform results

$$\begin{cases} Gmi\ (z) = Gmi\ \dfrac{(1-\alpha_m)}{(z-\alpha_m)} \\ \alpha_m = e^{\left(-\frac{Ts}{\tau_{mi}}\right)} \end{cases} \tag{3}$$

$$\begin{cases} Gdi\ (z) = Gdi\ \dfrac{(1-\alpha_d)}{(z-\alpha_d)} \\ \alpha_d = e^{\left(-\frac{Ts}{\tau_{di}}\right)} \end{cases} \tag{4}$$

In the canonic form,

$$\begin{cases} x_m(k+1) = \alpha_m.x_{mi}(k) + \alpha_d.x_{md}(k) + Gmi.(1-\alpha_m).u(k) + \\ \qquad Gdi.(1-\alpha_d).d(k) \\ y_m(k) = x_m(k) \end{cases} \tag{5}$$

Accounting the inputs of manipulated variable *u(k)* and a perturbation *d(k)*, the system response at (n+H) point becomes

$$\begin{aligned} y(n+H) &= \alpha_m^H.x_{mi}(n) + \alpha_d^H.x_{md}(n) + \\ &\sum_{j=0}^{H-1} \alpha_m^{H-1-j}.Gmi.(1-\alpha_m).u(j+n) + \\ &\sum_{j=0}^{H-1} \alpha_d^{H-1-j}.Gdi.(1-\alpha_d).d(j+n) \end{aligned} \tag{6}$$

The model output can be expressed as a sum of free (L) and forced (F) terms

$$y_m(n+H) = y_F(n+H) + y_L(n+H) \tag{7}$$

$$\begin{aligned} y_m(n+H) &= \alpha_m^H.y_{mi}(n) + \alpha_d^H.y_{md}(n) + \\ &Gmi.(1-\alpha_m^H)u(n) + Gdi.(1-\alpha_d^H).d(n) \end{aligned} \tag{8}$$

Therefore the control equation is obtained by the following steps

$$\varepsilon(n+H) = \varepsilon(n).\lambda^H \tag{9}$$

$$\lambda = e^{-\frac{3Ts}{TRBF}} \tag{10}$$

$\alpha_m^H.y_{mi}(n)$:

$\rightarrow$ Free responses

$\alpha_d^H.y_{di}(n)$:

$Gmi.(1-\alpha_m^H).u(n)$:

$\rightarrow$ Forced responses

$Gdi.(1-\alpha_d^H).d(n)$:

$$\begin{cases} \varepsilon(n) = c(n) - y_p(n) \\ \varepsilon(n+H) = c(n) - y_R(n+H) \end{cases} \tag{11}$$

$$\Rightarrow c(n) - y_R(n+H) = \lambda^H.(c(n) - y_p(n))$$

and considering

$$\Delta_p(H) = (c(n) - y_p(n)).(1-\lambda^H) \tag{12}$$

$$\begin{cases} \Delta_p(H) = \Delta_m(H) \\ (c(n) - y_p(n)).(1-\lambda^H) = y_m(n+H) - y_m(n) \end{cases} \tag{13}$$

then,

$$\begin{aligned} &(c(n) - y_p(n)).(1-\lambda^H) = \alpha_m^H y_{mi}(n) + \alpha_d^H y_{md}(n) + \\ &Gmi(1-\alpha_m^H)u(n) + Gdi(1-\alpha_d^H).d(n) - y_m(n) \end{aligned} \tag{14}$$

The control algorithm is given by

$$\begin{aligned} u(n) = &\frac{(1-\lambda^H)}{Gmi(1-\alpha_m^H)}(c(n) - y_p(n)) - \frac{\alpha_m^H}{Gmi(1-\alpha_m^H)} y_{mi}(n) \\ &- \frac{\alpha_d^H}{Gmi(1-\alpha_m^H)} y_{md}(n) - \frac{Gdi(1-\alpha_d^H)}{Gmi(1-\alpha_m^H)} d(n) + \frac{y_m(n)}{Gmi(1-\alpha_m^H)} \end{aligned} \tag{15},$$

which can be expressed as

$$\begin{aligned} u(n) = &K_0.\varepsilon(n) + K_1.y_{mi}(n) + \\ &K_2.y_{md}(n) + K_3.d(n) + K_4.y_m(n) \end{aligned} \tag{16}$$

naming

$$\begin{aligned} K_0 &= \frac{(1-\lambda^H)}{Gmi.(1-\alpha_m^H)} \qquad K_1 = \frac{-\alpha_m^H}{Gmi.(1-\alpha_m^H)} \\ K_2 &= \frac{-\alpha_d^H}{Gmi.(1-\alpha_m^H)} \qquad K_3 = \frac{-Gdi.(1-\alpha_d^H)}{Gmi.(1-\alpha_m^H)} \\ K_4 &= \frac{1}{Gmi.(1-\alpha_m^H)} \end{aligned} \tag{17}$$

Finally, if it is assumed that $d(n) = y_{md}(n) = 0$

$$\frac{U(z)}{\varepsilon(z)} = \frac{K_0.(z-\alpha_m)}{(z-1)} \tag{18}$$

As can be seen from (18) the controller transfer function has an implicit integrator which guarantees zero tracking error for step inputs

The forced response is calculated by assuming the input to the plant is related to base functions as are shown in Fig. 2. Typically these functions are polynomial types such as steps $B_1(i) = 1$; ramps $B_2(i) = i$ or parabolas $B_3(i) = i^2$. The choice of the basis functions defines the input profile and can assure a predetermined behavior.

$$u(n+i) = \sum_{K=1}^{Nb} \mu_K(n) UB_K(i) \tag{19}$$

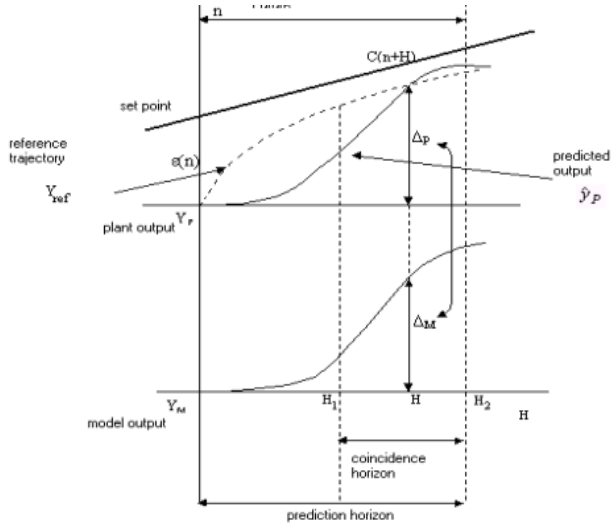

Fig. 1. PFC principles for design for one coincidence point.

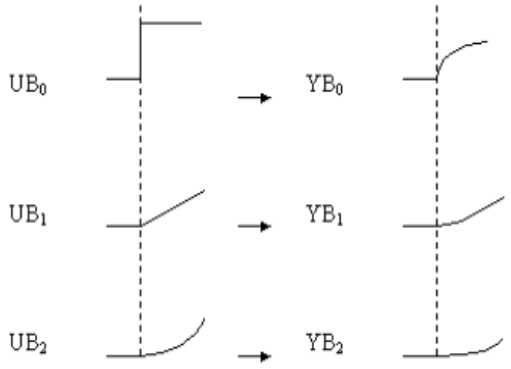

Fig. 2. base function for input and forced output calculations

For system with delay it must be estimated the error between plant and model at instant (n-Tdm) as is shown in Figure 3. There, Tdm is the time delay. Hence the predicted output of the plant is given by

$$\hat{y}_p(n) = y_m(n) + e_{0\,RET}(n) \tag{20}$$

$$e_{0ret} = y_{\Pr et} - y_{Mret} \tag{21}$$

where

$$\hat{\varepsilon}(n) = (c(n) - \hat{y}_P(n)) \tag{22}$$

Accounting considerations (20) to (22) the control algorithm for the system with delay is given by

$$\boxed{u(n) = K_0.\hat{\varepsilon}(n) + K_1.y_{mi}(n) + K_2.y_{md}(n) + K_3.d(n) + K_4.y_m(n)} \tag{23}$$

The parameters to be tuned for these controllers are: *coincidence point (H)* [sec]. C*losed loop time response* [TRBF, sec] of the reference trajectory. If control zone is applied *low and high* TRBF must be defined. The high value is applied when controlled variable is exactly at the set point. If it is going far from the set point but it is inside the allowed zone TRBF decreases linearly up to the limit of the zone where it reaches the lower value in order to drive the controlled variable inside the zone as quickly as possible. By using a control zone the parameter TRBF is moving linearly between those two extremes (low and high values).

Transition zone [%] set the allowed zone for the controlled variable expressed as ± n% with respect to set point value, c*onstraints to manipulated variable* are also included fixing maximum, minimum and variations for it.

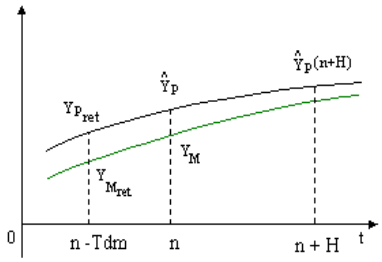

Fig. 3 prediction of the delayed response

3. CASE STUDY

The system studied here was obtained from (Galvez and Figueroa; 2000), who worked with two cascaded reactors. However, for simplicity reasons, only the first reactor is considered here. It consists of a constant-volume and density, cooled CSTR with a first order, irreversible reaction $A \rightarrow B$. While this model is quite simple it still contains most of the relevant issues surrounding an open- loop, non linear reactor. Referring to Figure 4, this system can be described by one component balance and one energy balance,

$$dC_A/dt = -k_0 e^{-T^*/T_1} C_A + \left(Fin_A/V_1\right)(C_{inA} - C_A) \tag{24}$$

$$\frac{dT}{dt} = k_1 e^{-T^*/T_1} C_A + \left(Fin_A/V_1\right)(Tin_A - T_1) + \left(Q_{jp}/\rho_p c_p V_1\right) \tag{25}$$

Accounting the energy balance for the jacket,

$$dT_J/dt = \left(F_{J0}/V_J\right)(T_{J0} - T_J) - \left(Qjp/\rho_j c_j V_j\right) \tag{26}$$

where the interchanged heat is given by:

$$Q_{JP} = \frac{U_a k_J F_{J0}(T_{J0} - T_1)}{(U_a + k_J F_{J0})} \tag{27}$$

F_{inA}, F_{J0} , F1, F_J [m3/seg] flows
C_{inA} ,C_A [mol/m3]: *concentrations*
T_{inA}, T_{J0}, T_1, T_J , T*[ºK]: *temperatures*
Q_{JP} = heat transferred [J/seg].

In Table 1 are given the nominal values for the principal variables of the system.

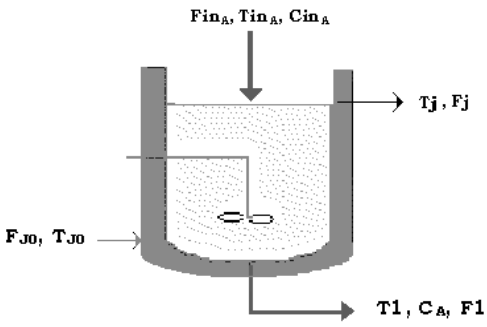

Fig. 4. CSTR model nomenclature

Table 1: reactor parameters and nominal values

Parameter	Value
V1: reactor volume	5 [m3]
V_J: jacket volume	1 [m^3]
ρ_P cp: density and heat capacity of the product	1[J/m3ºK]
$\rho_J c_J$: density and heat capacity of the cooler	1 [J/m3*ºK]
k_0: specific rate of reaction	2.7e8 [1/seg]
Ua: heat transfer capacity of cooling jacket	0.35 [W/ºK]
Dh	5 [ºK m^3/mol]
T*: activation temperature	6000 [ºK]
k_1= Dh k_0	1.35e9 [ºKm^3/seg mol]

4- CONTROL STRATEGIES

The control system must manipulate heat removal from the reactor, but what should be the measured (controlled) variable?. Temperature is a good choice as it has a close thermodynamic relation with heat so, for the four schemes evaluated here, reactor temperature is the selected controlled variable. The principal differences among the schemes are focused on the manipulated variables. In the four cases the principal controller is PFC, for its implementation was used the MATLAB library described in (Amue et al.2001).

Scheme I: the simplest method for cooling the CSTR is shown in Figure 5 where the reactor temperature is controlled by manipulating the coolant flow to the jacket.

Scheme II: in Figure 6 can be seen that here the manipulated variable is the set point of the coolant temperature which is cascaded to a heat exchanger control system. However here its dynamic was not considered in order to simplify the analysis.

Scheme III: in Figure 7 it can be seen one of the thermodynamic control strategy proposed here. In this case the manipulated variable is the enthalpy entering the jacket which defines, in an optimal way, the coolant flow and temperature set points which are cascaded to the heat exchanger .

Scheme IV: in Figure 8 is shown the proposed methodology. As the same as scheme III the enthalpy entering the jacket is the manipulated variable and defines the coolant flow and temperature which are cascaded for manipulating both the recycle and the fresh coolant streams valves. It is assumed that the coolant temperature at the input and output points of the jacket, To and Tj respectively are available or estimated. Therefore, Fo and F_R are calculated by applying a steady state mass and component mass balances around the mixer given by equations (28). This control structure acts in split range manner.

$$F_{J0} * T_{J0} = F_R * T_J + F_0 * T_0$$
$$F_{J0} = F_R + F_0 \qquad (28)$$

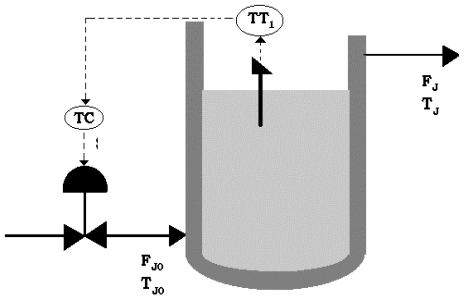

Fig. 5. Temperature CSTR control with scheme I

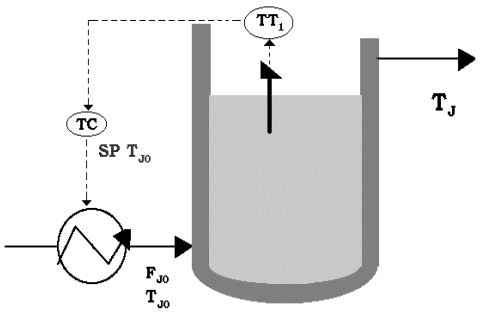

Fig. 6. Temperature CSTR control with scheme II

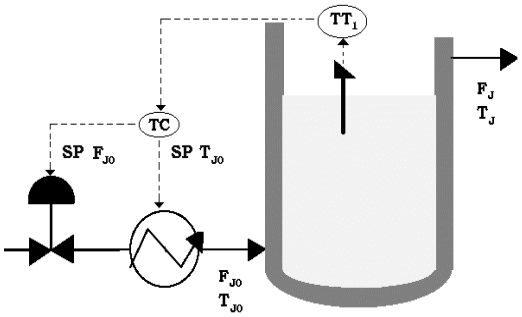

Fig. 7. Temperature CSTR control with scheme III

Note that in all cases the manipulated variable changes are defined by minimizing the IAE (Integral Absolute Error) moving one of the most important tuning parameters of the PFC, such as the closed loop time constant reference trajectory (TRBF). Only schemes III and IV consider thermodynamic control

where the coolant enthalpy is the manipulated variable. In scheme III the decision for choosing the best values for coolant flow and temperature was done optimally by applying sequential quadratic program (SQP) with restrictions. The steady state conditions which represent the nominal operation point are given in Tables 2 to 4.

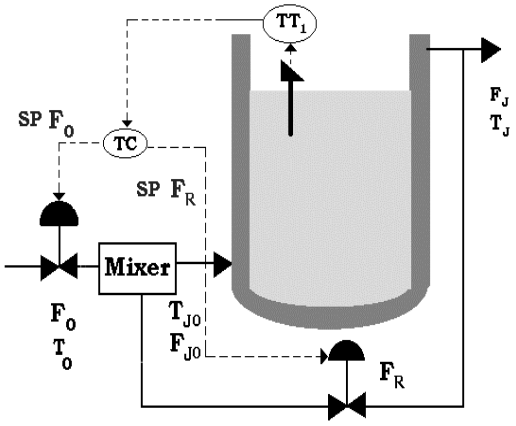

Fig. 8. Temperature CSTR control with scheme IV

5.APPLICATION RESULTS

Four strategies were tested for servo and regulator problem. In Figure 9 are presented the different dynamic responses for several perturbation on $T_{inA,}$ while Figure 10 shows the reactor temperature variations for several set point changes. Table 5 shows that for both servo and regulator problem scheme IV presents the lowest IAE values.

6. ANALYSIS OF THE ECONOMIC BENEFITS FOR EACH STRATEGY.

Typically a product is deemed acceptable if it is within the specification and unacceptable if it violates the specification. The normal procedure for establishing benefits for improved process control is based on steady state concepts. Here it will be used dynamic information for evaluating the economical benefits for each control strategy. Accounting the procedure presented by Latour (2000) where the distribution curves for regulation about the same average point for each strategy are analyzed.

In this work even though temperature was the controlled variable it is directly related with the quality of product. For the reaction considered here there is an optimal value (C_{BOPT} = 19.02 [mol/m^3]) and a rejected product when C_{BREP} = 18.99 [mol/ m^3]. In Figure 11 can be seen the distribution analysis for each scheme where number IV presents the lowest standard deviation, therefore the product is more uniform. Along with this studio and accounting an economic penalty for those strategies with spec violations, it can be assigned a real benefit for using each one. In Table 6 is presented the detailed calculation for the economic benefit obtained for each scheme. As in this case study a generic reaction was considered several assumptions were done in order to achieve a reasonable conclusion concerning on the real economic benefit when thermodynamic control is applied. It is considered that many aspects as feed cost, selling price and penalties for both excess or rejected quality were the same for all the schemes analyzed. So for comparison purposes it is assumed that this procedure is quite acceptable for defining "the best control strategy".

Table 2: nominal input variables to the reactor

Input variable	Value
C_{inA}	20 [mol/m3]
T_{inA}	300 [ºK]
F_{inA}	0.75 [m3/seg]

Table 3: nominal output variables to the reactor

Output variables	Scheme I, II and III	Scheme IV
C_A	1.3888 [mol/m3]	1.388 [mol/m3]
T_1	320.5862 [ºK]	320.5862 [ºK]
T_J	176.8006 [ºK]	165.294 [ºK]

Table 4: nominal manipulated variables for each scheme

Manipulated Variables	Schemes I, II and III	Sheme IV
F_{J0}	1.2 [m3/seg]	1.124 [m3/seg]*
F_R	---------	0.28 [m3/seg]
T_{J0}	120 [ºK]	116.431 [ºK]*
F_0	---------	0.832 [m3/seg]
T_0	---------	100 [ºK]

*inferred variables

Table 5 IAEs for servo and regulator problem using each scheme

Scheme	IAE for Servo behavior	IAE for Regulator behavior
I	105.0237	12.1921
II	186.1816	21.8679
III	100.4811	8.7129
IV	81.3983	4.127

7. CONCLUSIONS

In this work the thermodynamic control implemented with PFC was confronted with other most commonly control strategies applied to a CSTR system. Particularly considering the enthalpy as a manipulated variable and handling it by recycling the coolant demonstrated to be the best option under the assumptions given above. Both by performance index IAE and based on an economic analysis it

seems to be superior from the other alternatives studied here.

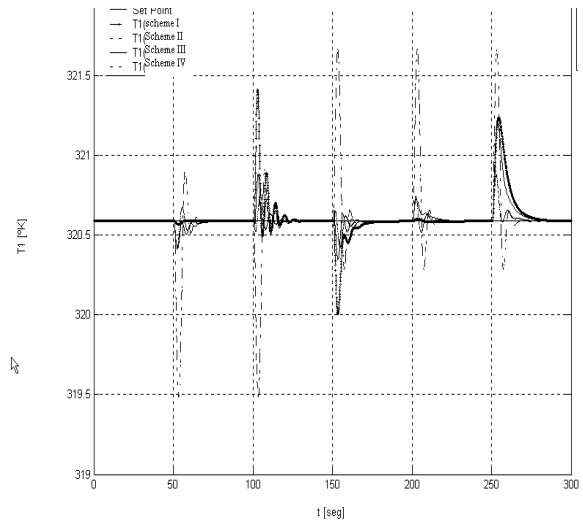

Fig. 9: dynamic responses for several perturbation on T_{inA} for each sheme

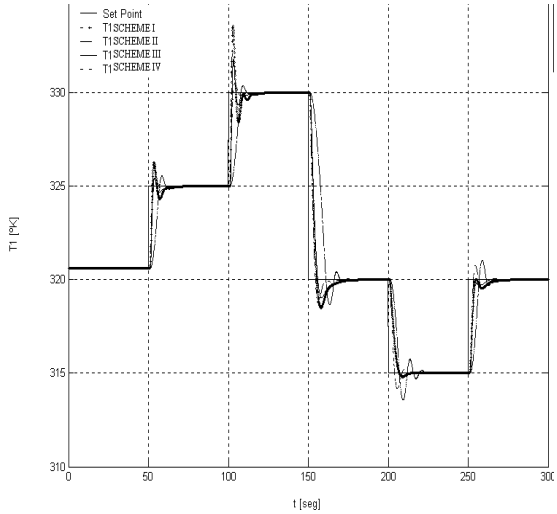

Fig. 10 reactor temperature variations for several set point changes for each scheme

$$SP = k_{PV} * F_1 * \overline{C}_B$$

Assuming that

$k_{PV} = 0.0002$ [\$/mol].

$F1=2700[m^3/h]$.

$\overline{C}_B$ [mol/m^3]: product mean value

.

$$C_0 = k_{C0} * F_{ina} * C_{ina} =$$

$$1e-4[\$/mol] * 2700\left[m^3/h\right] * 20\left[mol/m^3\right] \cong 5.5[\$/h]$$

$$L_{01} = k_1 * \Delta_{OPT} = k_{01} * F_{ina} * \left|\overline{C}_B - C_{BOPT}\right|$$

$k_{01}=0.01$ [\$/mol].

R: the reprocessing fraction

$$R = P(C_B \le \frac{\Delta_{REP}}{\sigma}) + 1 - P(C_B \le \frac{\Delta_{OPT}}{\sigma})$$

k2=10.

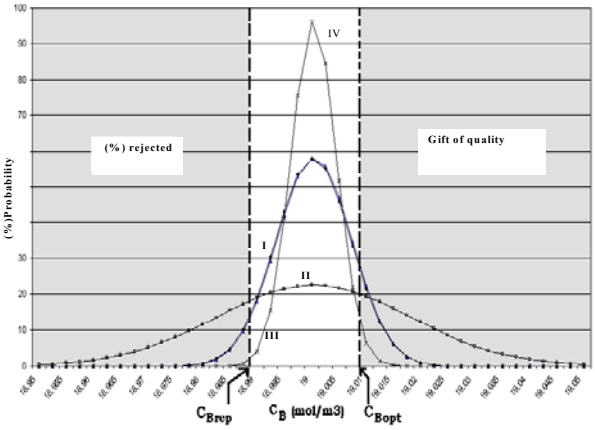

Fig. 11 Gaussian distribution curves for each scheme.

Benefit formula	Bi = SP - FC - K1*(Cbopt - Cb) - K2*R				
	Scheme I	Scheme II	Scheme III	Scheme IV	
Selling Price(SP)	10,261	10,261	10,260	10,260	[$/Hour]
Feed Cost(FC)	-5,500	-5,500	-5,500	-5,500	[$/Hour]
K1*(Cbopt - Cb)	-0,513	-0,540	-0,540	-0,540	[$/Hour]
K2*R	-0,640	-4,120	-0,690	-0,060	[$/Hour]
Benefit	3,608	0,101	3,530	4,160	[$/Hour]
x Hour/year				8000	[Hour]
Anual benefit	28.864,0	808,0	28.240,0	33.280,0	[$/year]

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