ANALYSIS OF SEVERAL CONTROL STRUCTURES ON AUTOREFREGRIGERATED REACTOR

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ABSTRACT

Autorefregirater reactor is a chemical reactor that uses latent heat to remove accumulation of heat from ex-thermal chemical reaction. It has been previously investigated that using temperature controller, the response of temperature towards disturbance of feed flow rate was found to be good and the process was controllable.

Several control structures in this paper were applied to this reactor and explored their behaviors towards disturbance from feed flow rate. These include product composition control, reaction rate control, and cascade control which are believed to give a better result than the conventional control structure. A change of 10% of feed flow rate was assumed. A comparison on the settling time, overshoot and deviation magnitude of the desired output was studied. Controller parameters were tuned according to Relay Feedback Test – Auto–Tuning Variation. The results show that temperature control yield better performance in terms of less overshoot and settling time, while product composition surprisingly gives inferior performance compared to the other one. The settling time for product composition control is 90.77 hours compared to 0.32 hours for temperature control. Minimum TAE for temperature control support the advantage of using this control structure. Deviation magnitude of the desired output appeared to be insignificant for all controller structures.

INTRODUCTION

Many processes can tolerate poorly designed control systems, but most chemical reactors will not. Some need a small load upset to break into oscillation sufficiently violent to ruin product, destroy catalyst and damage equipment. An exothermic reaction is one in which reaction may be unstable. Besides, an irreversible exothermic evolutes heat that is accumulated on the reactor and temperature runaways can occur. This presents a serious problem in scaling up chemical reactors. Cheung and Luyben (1979) have quantitatively showed that controllability on exothermic reactor decreases when reactor size increases. The higher capacity of the reactor the larger the heat generation. On a jacketed reactor, the heat transfer area is limited by the geometry of the reactor vessel. The ratio of heat transfer area (varies with $A^D$) to reactor volume (varies with $D^3$) decreases as the reactor gets bigger.

Since the size of the heat exchanger is not dependent on the size of the reactor, the scale up problem is avoided. Evaporative cooling (autorefrigeration) is one alternative for this heat exchanger type. Many industrial reactors use it.

PROCESS CONDITION AND REACTOR DESIGN

Autorefregirater reactor uses latent heat to remove accumulation of heat. Luyben (1999) has shown the effect of the fundamental process and design parameters on stability. This heat removal technique is limited to liquid phase reaction where temperature/pressure permit the liquid in the reactor to operate at its bubble point. Vapor from the reactor flows to a heat exchanger where it is condensed, and the liquid is returned to the reactor. The condenser operates at bubble point temperature of the vapor mixture from the reactor. The condenser also operates at lower pressure than the reactor since there must be pressure gradient to drive the vapor from the reactor to the condenser. The typical result is a significantly lower temperature in the condenser than in the reactor. This affects the required coolant temperature and water flow rate on condenser to release heat to surrounding.

To explore the dynamics and control of autorefregirated reactors, we select a specific reaction system that is typical of many industrials reaction systems. We use the system that has been developed (Luyben, 1999).

The second order irreversible exothermic reaction is $A + B ⇌ C$, with a Arrhenius temperature dependence. Specific reaction rate is $k$ (mole mole$^{-1}$s$^{-1}$)(total H2O/ mole), (mass fraction A).( mass fraction B) at 175°C. Assuming there is no component C in the fresh feed stream, ideal vapor-liquid equilibrium, and the composition of the liquid condensed in the condenser is the same as that of the vapor learning.
from the reactor. Bubble temperature dependence on vapor pressure is calculated from Antoine equation.

The vapor flow from the reactor to the condenser by pressure gradient is given by

$$ V = K_v \sqrt{P_R - P_C} \quad (1) $$

where $K_v$ is the vapor hydraulic constant.

The driving force for liquid flow from the condenser back to the reactor is by gravity, a height of liquid is built up in the liquid return line to provide the pressure driving force to get the liquid to flow from the condenser, which is at a lower pressure, into the reactor at higher pressure. It's given by

$$ L_p = K_h \left( \frac{h_R - h_C}{h_C} \right) \quad (2) $$

where $K_h$ is the liquid hydraulic constant.

Process condition on the reactor:
- $P = 50$ lb/in$^2$
- $C_L = 75$ Btu/lb$^\circ$F
- $T_R = 135^\circ$F
- $F_0 = 5.000$ lb
- $Z_{in} = 0.65$
- $Z_{out} = 1.0$
- $Z_{cond} = 1.0$
- $Z_{cool} = 1.0$

Figure 1. Autorefrigerated Reactor with Temperature Control Structure

Luyben (1999) has shown that the higher the conversion, the lower the activation energy, and the larger the condenser area than common heuristics would suggest were more helpful for control. We can develop reactor condition by using the values which are 90 % of the conversion, 30,000 Btu/lb mole of the activation energy, and a value of the heat transfer area for 26.3$^\circ$F of the temperature gradient. The pressure gradient between reactor and condenser is 1.0 psia. The cooling water coming out from the condenser is at 110$^\circ$F.

The steady state values are

| Composition of A reactant ($Z_a$), mole fraction | 0.2437 |
| Composition of B reactant ($Z_b$), mole fraction | 0.6756 |
| Temperature of reactor ($T_R$), $^\circ$F | 175 |
| Pressure of reactor ($P_R$), psia | 61.547 |
| Temperature of condenser ($T_C$), $^\circ$F | 136.2 |
| Heat liquid in reactor ($h_R$), ft | 3 |
| Flow rate of cooling water ($F_{cool}$), ft$^3$/hr | 329.55 |
| Temperature of cooling water in condenser ($T_{cool}$), $^\circ$F | 110 |

and specification of rector design are

| Table 2. Design of Autorefrigerated Reactor |
| Reactor hold up, ft$^3$ | 73.9 |
| Heat transfer area, ft$^2$ | 208.6153 |
| Specification of condenser |
| 1. Shell and Tube | 1-2 |
| 2. Diameter of tube, in | 3/4 |
| 3. Diameter of shell, in | 12 |

**PROCESS DYNAMIC AND SIMULATION**

In this section a rigorous non linear mathematical model of an autorefrigerated reactor is used (Luyben, 1999). The assumptions are

1. The reactor is perfectly mixed, the vapor boiling off the reactor is in ideal vapor-liquid equilibrium with the liquid phase, and the composition and pressure dynamics of the vapor phase in the reactor are neglected, this means that the pressure in the reactor dependence on temperature and composition in the reactor. It also means that the composition of the vapor stream to the condenser is the same as the composition of the vapor boiling off the liquid phase in the reactor.

2. The composition and thermal dynamics in the process side of the condenser are neglected and the condenser temperature is calculated from an iterative bubble point temperature calculation with the condenser pressure and the composition of the liquid phase in the condenser. The pressure in the condenser is calculated from a total mass balance, looking at the difference between the vapor flowing into the condenser and the liquid being condensed. Perfect gas behaviour is assumed. The temperature and liquid composition in the return line is the same as the temperature and liquid composition in the condenser.
3. The cooling water on the cold side of the condenser is perfectly mixed and the heat transfer rate
\[ Q_c = U \Delta T \text{ (Tc-Tco)} \] (3)
The dynamic equations are
\[ R = \alpha e^{-\frac{R(T-460)}{460}} V \frac{dZ_A}{dt} Z_B \] (4)
\[ \frac{dV}{dt} = \frac{F_0 + L_p \cdot V - P \cdot R}{R_B} \] (5)
\[ \frac{d(V_kZ_k)}{dt} = -f_{zo} Z_o \cdot L_p \cdot x_p \cdot V \cdot Y_k - P \cdot Z_k - R \] (6)
\[ \frac{d(V_kZ_A)}{dt} = f_{zo} Z_0 + L_p \cdot x_p \cdot V \cdot Y_k - P \cdot Z_A - R \] (7)
\[ \frac{d(V_kZ_B)}{dt} = \frac{C_p M_k F_0 T_0 + C_p M_c L_p T_c - \Delta H_k}{C_p M_k \cdot T_x - \Delta H_k} R \] (8)
\[ V \frac{d(P_x)}{dt} = V - L_c \] (9)
\[ \rho \cdot A_t \cdot \frac{d(h)}{dt} = \frac{1}{L_c - L_p} \] (10)
\[ \rho_{\max} C_p \max \frac{d(T_{CC})}{dt} = \rho_{\max} C_p \max f_{CC}(T_{G0}-T_{CC}) \] (11)
These seven non-linear ordinary differential equations are numerically integrated. We can complete it by using control structure and develop closed loop model system.

**COMPARISON OF FOUR CONTROL STRUCTURES**

Reactor volume is controlled by level controller which has a dimensionless gain \( K_C = 4 \). The control equation for level controller is
\[ P = P^* = K_C (H_{\text{hit}} - H_{C}) \] (12)
Value of product rate is spanned of twice the steady state design value. The other controller uses cooling water as the manipulated variable. Value of cooling water is spanned of twice too. Assume all control valves have linear installed characteristics. Input disturbance was assumed to be feed flow rate. Lundén (1999) has developed temperature control structure (Figure 1). In this section we develop other control structures that are composition control (Figure 2), cascade control for product composition (primary loop) and reactor temperature (secondary loop) (Figure 3), and computationally reaction rate control by using the temperature of reactor and the product composition signals (Figure 4). Level control uses Proportional Only Control Mode.
The control equation for each structures is:
1. Temperature controller
\[ F_C = F_{CC}^* + K_{C_t} (T_{CC} - T_h) + 1/L_t \int (T_{CC} - T_{CC0}) \] (13)
2. Product composition controller
\[ F_C = F_{CC}^* + K_{C_t} (Z_{CC} - Z_{CC0}) + 1/L_t \int (Z_{CC} - Z_{CC0}) \] (14)
3. Cascade control of temperature and product composition
This cascade structure takes the product composition as the master control and the temperature as the slave one. Slave controller uses proportional only mode controller to get a simple response and master controller uses proportional-integral-mode controller to upgrade response quality and to reduce offset effect at slave loop.
\[ T_{CC0} = K_{C_t} (C_{CC} - Z_{CC0}) + 1/L_{C_t} \int (Z_{CC} - Z_{CC0}) \] (15)
Slave:
\[ F_C = F_{CC}^* + K_{C_t} (T_{CC0} - T_h) \] (16)
4. Rate reaction control by computational methods
This control structure holds product composition value that is based on reaction rate (eq. 4). Therefore we modify several component of rate reaction equation based on steady state.
\[ (Z_h Z_{h0})_{\text{Ct}} = 0.24733 Z_e^2 - 0.50477 Z_e + 0.24742 \] (17)
\[ C_{\text{CC}0} = 1.0705 10^{15} \text{mol}^{-1} \text{m}^{-3} \text{mol}^{-1} \text{L}^{-1} \text{K}^{-1} \] (18)
\[ V \frac{d(V_kZ_k)}{dt} = (10.23193)(1480873+H_k)(1+Ze) \] (19)
We develop rate reaction equation to be new formula as the computed rate reaction.
\[ R_h = 0.11 Z_e^2 - 0.51 Z_e + 0.25 \] (20)
\[ (10.23193)(1480873+H_k)(1+Ze) \] (21)
which the reactor temperature, product composition and level are signal inputs. The controlled variable is designed to be dependent on product flow rate.
\[ Z_e = R_h (C_{\text{CC}0}^2) \] (21)
The product flow rate is an input signal. The control equation is
Fcc = Fcc⁰ + Kc⁰com (Zc^SET - Zc^COM) +
1 / Fc⁰com \int (Zc^SET - Zc^COM) \, dt \quad (22)

Exothermic reactor is non-linear open loop system (Luyben, 1990). It's tuned for each structure by using Relay Feedback Test-Auto Tuning Variation (Luyben, 1990). Control gain and integral time are calculated using the Tyreus-Luyben tuning rules (Tyreus & Luyben, 1992). Evaluation of performance control structures by total error relatively from each control structure set point is given by

IAE_N = \int \left| N^\text{SET} - N \right| dt / N^\text{SET} \quad (23)

where N is output of controlled variable from each controller structure.

Figure 2. Product Composition Control Structure

Figure 3. Cascade Control Structure

RESULT AND CONCLUSION

Evaluation of control structure emphasizes on controller ability to give the best performance on overshoot, settling time, deviation magnitude of the desired output and minimum value for total error.

Temperature Control

In this structure, temperature is kept constant at 175°F. A change of 10% of feed flow rate was assumed. Composition of C product decreases as far as 1.07% from required value 0.6897. The reactor temperature overshoots to 0.68% from 175°F. Response oscillation with Kcₕ 5.1 and T₁₁ 0.18 is relatively high but it's faster to get new steady state (0.52 hours). Temperature response is shown on Figure 5 while composition of C product response is on Figure 6. IAE_N value is 20.75%.

Figure 4. Reaction Rate Control Structure

Fig. 5. Response of Reactor Temperature
Product Composition Control

Control is used to keep composition of C product at set point 0.6807 (Figure 8). It makes reactor temperature increase 1.34 % from the set point, 175 °F (Figure 7). Oscillation response is not as high as temperature control, but it needs longer time to get new steady state (90.77 hours). Responses by $K_C$, 0.08 and $T_D$, 1.72 are shown on Figure 8, that composition overshoots to 5.28 % from 0.6807. IAE value is 1.35108 %.

Cascade Control for The Product Composition-Temperature

This cascade control structure puts composition of C product control as the master control, while temperature control as the slave one. This control structure improves performance of composition control by reducing the settling time (1.84 hour) to obtain new steady state. The composition overshoots drops to 0.9 % (Figure 9). Product composition is the set point and temperature reactor increases up to 1.25% (Figure 10). IAE value is 95.11 %. $K_C$ 1.56, $T_D$, 0.58 and $K_C$ 1.25 were given as control parameter values.
Computational Control for The Reaction Rate

The response with $K_C\cos$ 3.32 and $\tau_{CM}$ 0.11 shows that the temperature increase to 1.34% (Figure 11) and the composition can hold at the set point (Figure 12). This control structure improves response of composition control structures. It reduces the settling time to 1.13 hours, drops the composition overshoot to 1.34% and improves the oscillation response. IAE value is 138.56 %.

![Fig. 11. Response of Reactor Temperature](image)

![Fig. 12. Response of Product Composition](image)

Controller performance are evaluated by values of overshoot, settling time and deviation magnitude of the temperature or composition uncontrolled output variable and evaluation error are evaluated by IAE method. Set point value is tolerated for 0.05 % error.

From the four control structures, temperature control indeed has the best performance in terms of less overshoot and settling time as given by Luyben. Minimum IAE for temperature control supports the advantage of using this control structure. The cascade control and rate reaction control improve performance of the composition control by eliminating overshoot, settling time and IAE value. Deviation magnitude of the desired output appeared to be insignificant for all controller structures.

<table>
<thead>
<tr>
<th>Control Structures</th>
<th>Overshoot (%)</th>
<th>Settling Time (hour)</th>
<th>Deviation Magnitude (%)</th>
<th>IAE (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature control</td>
<td>0.6845</td>
<td>0.32</td>
<td>1.0741</td>
<td>20.75</td>
</tr>
<tr>
<td>Product composition</td>
<td>5.2801</td>
<td>90.77</td>
<td>1.3445</td>
<td>1351.08</td>
</tr>
<tr>
<td>Cascade control</td>
<td>0.9025</td>
<td>1.84</td>
<td>1.2462</td>
<td>95.17</td>
</tr>
<tr>
<td>Computational control</td>
<td>1.3388</td>
<td>17.13</td>
<td>1.3381</td>
<td>138.56</td>
</tr>
</tbody>
</table>

NOMENCLATURE

- $A_H$: Heat transfer area ($ft^2$)
- $A_p$: Cross sectional area of liquid pipe ($ft^2$)
- $C_P$: Heat capacity (btu/lb$^\circ$F)
- $E$: Activation energy (btu/lbmole)
- $F_0$: Fresh feed flow rate (lbmole)
- $F_{C_c}$: Cooling water flow rate ($ft^3/h$)
- $F_{C_c}^*$: Steady state cooling water flow rate ($ft^3/h$)
- $g$: Gravity conversion (lb/ft$^3$)
- $h$: Height of liquid in return pipe (ft)
- $H_L$: Liquid hold up in reactor (ft)
- $H_{L,sp}$: Liquid hold up set point (ft)
- $\Delta H_r$: Reaction heat enthalpy (Btu/lbmole)
- $\Delta H_L$: Latent heat enthalpy (Btu/lbmole)
- $IAE_r$: Relative integral absolute error
- $K_F$: Gain control
- $K_{C,c}$: Gain control of cascade structure
- $K_{C,cm}$: Gain control of computed variable control
- $K_{L,sp}$: Gain control of level
- $K_{L,T}$: Gain control of temperature
- $K_{C,2}$: Gain control of composition
- $L_C$: Liquid hydraulic constant (lbmole/hour psi$^{-1}$)
- $L_c$: Vapor hydraulic constant (lbmole/hour psi$^{-1}$)
- $L_P$: Liquid flow rate from condenser (lbmole/hour)
- $M_e$: Molecular weight in condenser (lb/mole)
- $M_{c}$: Molecular weight in reactor (lb/mole)
- $M$: Molecular weight in reactor (lb/mole)
- $N$: Control variable value
- $N_{SET}$: Control variable set point value
- $P$: Product flow rate from reactor (lbmole/h)
- $P_C$: Condenser pressure (psi)
- $P_R$: Reactor pressure (psi)
- $Q_c$: Heat transfer rate (btu/h)

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$R$ Gas law constant (1.99 Btu/lb-mole °R or
1545/144 psia·ft³/lb-mole °R)
$t$ Time (h)
$T_c$ Condenser temperature (°F)
$T_{c,ave}$ Average condenser temperature (°F)
$T_{cool}$ Temperature of outlet coolant (°F)
$T_{in}$ Temperature of inlet coolant (°F)
$T_{off}$ Temperature of fresh feed (°F)
$T_d$ Temperature in reactor (°F)
$T_{X,ave}$ Temperature reactor set point of cascade
structure (°F)
$T_{X,sp}$ Temperature reactor set point (°F)
$U$ Overall heat transfer coefficient
(Btu/ft²·°F)
$V$ Vapor flow to condenser (lb mole/hour)
$V_e$ Effective vapor volume (ft³)
$V_b$ Reactor volume (lb mole)
$V_{shell}$ Shell side volume (ft³)
$X_{c,i}$ Liquid composition in condenser (mf)
$X_p$ Liquid composition in return pipe (mf)
$Y_i$ Vapor composition leaving reactor (mf)
$Z_{com}$ Composition set point (mf)
$Z_p$ Liquid composition in reactor (mf)
$Z_{0}$ Fresh feed liquid composition (mf)
$\alpha, \beta$ Arrhenius constant
$\rho$ Liquid density (lb/ft³)
$\tau_{X,sp}$ Integral time of cascade control (minute)
$\tau_{c,sp}$ Integral time of computed variable control
(minute)

**SUBSCRIPT**

**COM** Computed variables based on measured
variables

**i** Component of I

**REFERENCE**

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