



Model to Predict a Ratio Control of Hydrocarbon Acid and Water in a Packed Bed Reactor

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Abstract

Model development was carried out to examine the ratio of hydrochloric acid gas and water in a packed bed reactor. The research predicted increase in output with increase in time, revealing the effectiveness ratio control of hydrochloric acid separation from water using absorption column mechanism. The density of the products played an active role in the separation process as well as in control action function. The developed model can be applied to monitor, predict and simulate the degree of separation when hydrochloric acid gas is subjected into absorption column in the presence of water medium in a packed bed reactor. Increase in output response was observed with increase in time. The variation in output response was attributed to the variation in operating time. The mathematical model developed was simulated using Matlab software to monitor, predict and simulate the output response hydrochloric acid mixture with water in a packed bed reactor. The result obtained revealed effectiveness in separation is dependent of contact time as well as concentration of the both materials.

Keywords: Model, predict, ratio control, hydrochloric acid gas, water, packed bed reactor.

INTRODUCTION

Control is considered to be an important function that enhanced monitoring in terms of product composition and characteristics as well as the behaviour of a given process. In instrumentation the functional parameters that controls the system is monitored by checking the dependent and independent variables including other useful components that will enhance the efficiency of the process [1, 2].

On those processes of a packed bed reactor include the mechanical, chemical, instrumentation etc. and the concentration of the products which is hydrochloric acid gas and water [3]. The effectiveness in the removal of phenol from non-volatile liquid solvent has been studied as well as the removal of

solute from gas substance such as hydrochloric acid gas using absorption mechanical has been reported using vertical operation of a cylindrical column [4]. The packed bed reactors create a surface area for both liquid and gas contact which enhances mass transfer in both streams [5]. Investigation conducted showcase the different types of reactors which are useful in the separation of hydrochloric acid gas from water based on properties of both samples [6–9].

The properties of hydrochloric acid gas reveals colorless, temperature of 15°C, freezes -114°C, gas soluble in water 20°C, possess the ability to dissolve in water [10]. The application of absorption to control hydrochloric acid gas mixture with water by considering the dynamic and control

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mechanism has been revealed in this work as functional components were integrated in the simulation of the developed model [11].

The control set point play an active role in control action, dynamics, lay time, dependent variables, independent variables, as well as stability of the control action [11].

MATERIALS AND METHODS

The flow diagram showcase in Figure 1 demonstrates a simple ratio control.

Overall Mole Balance

The overall mole balance equation describing the process is expressed as shown equation (1) below

$$Gm (y1 - y2) = Lm (x1 - x2) \quad (1)$$

Equation (1) define the liquid and the gas phase contact in the absorption column.

Diameter of Absorption Column

The diameter of absorption column can be illustrated in terms of function of density gas liquid flow rate as well as density of fluid on liquid and flow rate of the gas. The mathematical expression of this given process can be written as:

$$f_{lv} = \frac{lm}{Gm} \sqrt{\frac{P_g}{P_l}} \quad (2)$$

Height of Absorption Column

In the packed bed reactor, the height of the absorption column can be evaluated using the equation showcased in equation (3) and (4) as that is for the upper region.

$$Gm (y1 - y2) = Lm(x1 - x2) \quad (3)$$

$$x2 = x1 + \frac{Gm}{Lm}(y - y1) \quad (4)$$

The equation (3) and (4) illustrates the mass transfer coefficient and expressing the height with respect to ordinary differential given the expression in equation (1).

$$Gm \times dy \times A = KG ap(y - ye) \times Axdn \quad (5)$$

The in the lower region, the mathematical expression can be written as

$$h = \int_0^h dn = \frac{-Gm}{kGap} \int_{y1}^{y2} \frac{dy}{y - ye} \quad (6)$$

The process plant and the various steps and control measures are demonstrated in Figure 2.

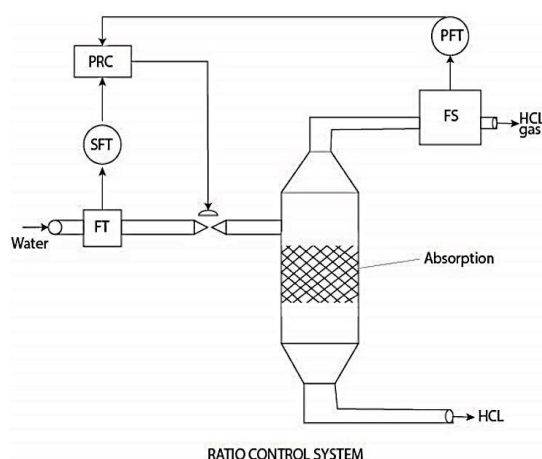


Figure 1. Diagram of a simple ratio control system [1].

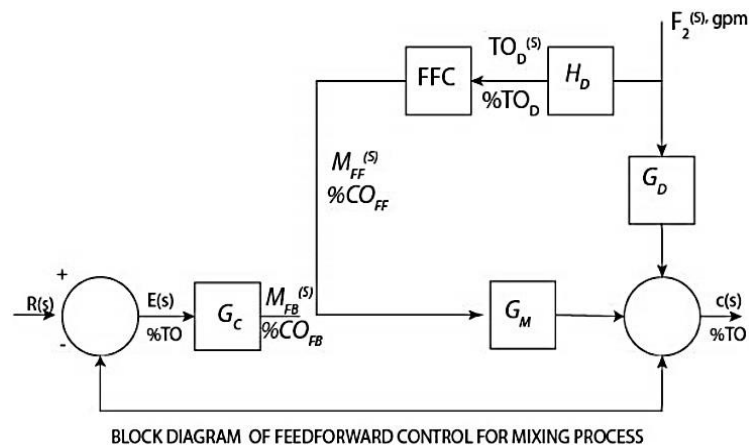


Figure 2. A simple feed forward control for mixing process [4].

The Control Strategies

The possible commonly used control actions are PD, DI and PID to monitor, predict and simulate the parameters of interest in a process plant as shown in Figure 2.

Proportional Integral Controller (PI)

The mechanism in terms of control of PI helps in eliminating errors that could have arisen on the steady state process. Therefore the mathematical expression for this process is given as:

$$P = Kc E_{(t)} + \frac{kc}{ti} \int_0^t E_{(t)} dt + ps \quad (7)$$

τ_1 is the integral time constant

$$p-ps = kc E_{(t)} + \frac{kc}{ti} \int E_{(t)} dt \quad (8)$$

$$p_{(s)} = kc E_{(t)} + \frac{kc}{c1} \frac{E_{(s)}}{s} \quad (9)$$

$$\frac{p_{(s)}}{E_{(s)}} = k_c + \frac{kc}{ti} \quad (10)$$

Therefore the transfer function of proportional integral controller is

$$G_{(s)} = k_c \left(1 + \frac{1}{c1s} \right) \quad (11)$$

Mechanism of Transfer Function

The equation (12) illustrates the mathematical expression of a simple mechanism of transfer function of process plant.

$$H_{(s)} = \frac{To(S)}{P} = \frac{kT}{T_{Ts}+1} \quad (12)$$

And the orifice is influence with differential pressure of the flow thus, the proportional to volumetric flow rate in which the differential pressure contributes on the characteristics and behaviour of the system, hence.

$$h \propto f^2 \quad (13)$$

Equation (13) described the signal (output) in terms of change in pressure with change in volumetric flow. The gain experience can be expressed as:

$$KT = \frac{\phi}{df} = \frac{2(100)}{f(max)^2} f \quad (14)$$

Transfer Function of Control Action

Final control played an active role in controlling the mechanism of the process plant by monitoring the variables as stated. The various equation illustrated below in equation (15) and (16) as well as the flow transmission showcased in equation (17).

$$Gv(s) = \frac{F(s)}{M(s)} = \frac{Kv}{Tvs+1} \quad (15)$$

$$Gv(s) = \frac{f(s)}{M(s)} = \frac{kv}{Tvs+1} \quad (16)$$

Flow transmitter is presented in equation (17) as:

$$Hs = \frac{KT}{Tts+1} \quad (17)$$

Feed Forward Control Loop

The Figures 2 was used to demonstrates a simple feed forward control for mixing process and the mathematical expression presented below.

The transfer function equations are stated below as:

$$\frac{Cv(s)}{Dm(s)} = \frac{Gv(s)Gp(s)Gffs(s)+Gd}{1+Gv(s)Gp(s)GC(s)} \quad (18)$$

$$Gff(s) = \frac{-Gd(s)}{Gp(s)} \quad (19)$$

$$\frac{Cv(s)}{Mv(s)} = Gp(s) = \frac{Kpe^{-es}}{Ts+1} \quad (20)$$

$$\frac{cv(s)}{Dm(s)} = Gd(s) = \frac{Kde^{-\theta ds}}{Tds+1} \quad (21)$$

$$Gff = \frac{Mv(s)}{Dm(s)} = \frac{-Gd(s)}{Gp(s)} = k_{ff} \left(\frac{T_{1ds+1}}{T_{1gs+1}} \right) e^{-\theta ff} \quad (22)$$

$$\frac{CV(s)}{Dm(s)} = \frac{\frac{-Kv}{Tvs+1} \times \frac{Kpe^{-\theta s}}{Ts+1} \times k_{ff} \left(\frac{T_{1ds+1}}{T_{1gs+1}} \right) e^{-\theta ff} + \frac{Kde^{-\theta ds}}{Tds+1}}{1 + \frac{Kv}{Tvs+1} \times \frac{Kpe^{-\theta s}}{Ts+1} \times k_{ff} \left(\frac{T_{1ds+1}}{T_{1gs+1}} \right) e^{-\theta ff} \times \frac{Kc(T_{1s+1})}{T_{1cs}}}$$

Solving the using Laplace transformation by evaluating the numerator

$$\frac{Kv \times Kpe^{-\theta s} \times k_{ff} (T_{1ds+1}) e^{-\theta ff} (T_{1dsr}) + Kde^{-\theta ds} (T_{vs+1}) (T_{s+1}) (T_{1gs+1})}{(T_{vs+1}) (T_{s+1}) \times (T_{1gs+1}) (T_{1ds+1})} \quad (24)$$

Evaluating the denominator we have

$$1 + \frac{(Kv)(Kpe^{-\theta s}) \times k_{ff} (T_{1ds+1}) e^{-\theta ff} \times Kc(T_{1s+1})}{(T_{vs+1}) (T_{s+1}) (T_{1gs+1}) (T_{1s})} \quad (25)$$

$$C_v = \frac{T_1(s + e^{-t}(ke^{-\theta}))}{1 + K_c} \quad (26)$$

RESULTS AND DISCUSSION

The result obtained from the simulation program is demonstrated below:

Simulation

```
function [tp,yp] = rk4sys2(dydt,tspan,y0,h)
% [t,y] = rk4(dydt,tspan,y0,h):
% uses the fourth-order Runge-Kutta method to integrate an ODE
```

```
% input:
% dydt = name of the M-file that evaluates the ODE
% tspan = [ti, tf] where ti and tf = initial and
% final values of independent variable
% y0 = initial value of dependent variable
% h = step size
% output:
% t = vector of independent variable
% y = vector of solution for dependent variable
n=length(tspan)
ti = tspan(1);
tf = tspan(n);
if n==2
    t = (ti:h:tf)';
    n = length(t);
    % if necessary, add an additional value of t
    % so that range goes from t = ti to tf
    if t(n)<tf
        t(n+1) = tf;
        n = n+1;
    end
else
    t=tspan
end
tt=ti;y(1,:)=y0;
np=1;tp(np)=tt;yp(np,:)=y(1,:);
i=1;
while (1)
    tend=t(np+1);
    hh=t(np+1)-t(np);
    if hh>h,hh=h,end
    while (1)
        if tt+hh>tend,hh=tend-tt; end
        k1=dydt(tt,y(i,:))
        ymid=y(i,:)+k1'*(hh./2)
        k2=dydt(tt+hh/2,ymid)
        ymid=y(i,:)+k2'*hh/2;
        k3=dydt(tt+hh/2,ymid)
        yend=y(i,:)+k3'*hh;
        k4=dydt(tt+h/2,yend)
        phi=(k1+2*(k2+k3)+k4)/6;
        y(i+1,:)=y(i,:)+phi'*hh;
        tt=tt+hh;
        i=i+1;
        if tt>=tend, break,end
```

```

end
np=np+1;tp(np)=tt;yp(np,:)=y(i,:);
if tt>=tf,break,end
end
function [dcvdt] = Year4(t,cv)
dcvdt=0
tau=5;
s=2
kc=8
k=9
dcvdt=tau*(s+k*exp(-2*t))/(1+kc)
end
%CALLUP
clear
clc
h=0.2
tspan=[0:h:12]
Cv0=0
[t,cv]=rk4sys2(@Year4,tspan,Cv0,h)
t=t'
table(t,cv)
plot(t,cv,'-*b')
xlabel('Time(s)')
ylabel('Output')

```

Figure 3 demonstrates the relationship between the output response and the time. The variation in the output response could be attributed to the variation in time. The simulation was run using the mathematical model stated in equation (26) and the mathematical equation is given as

$C_v = \frac{T_1(s + e^{-t}(ke^{-\theta}))}{1 + K_c}$. The output response was simulated by incremental increase in time as the response output increased linearly.

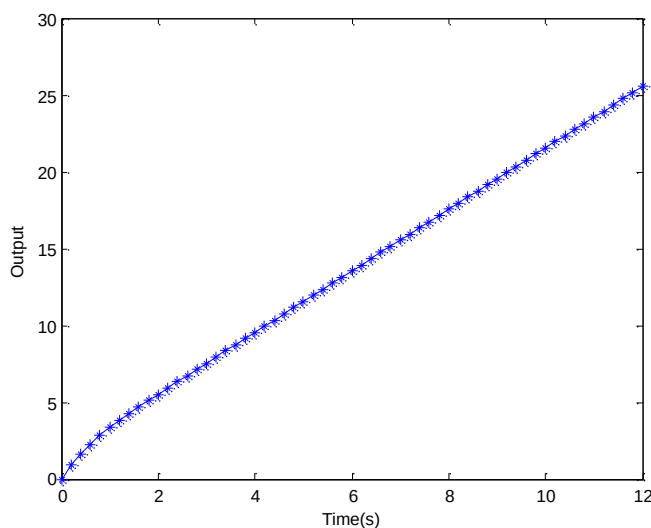


Figure 3. Graph of Output Response versus Time.

CONCLUSION

The following conclusion was drawn from the study as shown below:

- (i) The ratio control hydrochloric acid gas and water in absorption column is more effective when feed forward control mechanism is used in the packed bed reactor.
- (ii) The output signal is linear with increase in time
- (iii) The most effective control mechanism is when the feed forward and feed backward control action is installed in the packed bed reactor for the absorption process of hydrochloric acid gas separation with water medium.
- (iv) The research work demonstrates the mechanism of separation of gas phase from liquid phase using absorption column.

Nomenclature

G_m and L_m are the molar flow rates of the gas and liquid, respectively kmole/s

y_1 ; y_2 are the inlet and outlet concentrations of the solute in the gas, mole fraction

x_1 , x_2 are the outlet and inlet concentrations of the solute in the liquid mole fraction.

P_G is density of gas (HCl)

L_m = liquid flow rate

P_l is density of liquid (H₂O)

G_m = gas flow rate

A is the cross sectional area of the column, represents the packing area per volume

K_G is the overall gas phase mass transfer coefficient

y is the mole fraction in the bulk of gas and y_e is the mole fraction that the gas would have if it were in equilibrium with the liquid p is the total pressure which is constant.

b = output signal in % TO

f = volumetric flow

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