

Modelling and Control of a Diesel Hydrotreating Process

Zeyad M. Ahmed¹, Gurashi A. Gasmelseed²

¹Jazan University, Faculty of Science and Engineering, Saudi Arabia

²University of Science and Technology, Faculty of Engineering, Department of Chemical Engineering, Sudan

Abstract: The application of control theories to design the control of a planned or existing process or operation is always performed by blind methods such as trial and error or Zeiglar-Nichols method. The aim of this paper is to apply mathematical models and control theories to design control system of a diesel hydrotreating process. Understanding process dynamics (how process variable change with time) are important to determine the process modeling and process control. In this paper the process dynamics of Diesel hydrotreating unit were explored and reviewed some mathematical tools for solving the resulting process modelling and control.

Keywords: Modelling; Control; Diesel; Hydrotreating

1. Introduction

Hydrotreating is an established refinery process for reducing sulphur, nitrogen and aromatics while enhancing Cetane number, density and smoke point. The refining industry's efforts to meet the global trend for more-stringent clean fuels specifications, the growing demand for transportation fuels and the shift toward diesel mean that hydrotreating has become an increasingly important refinery process in recent years. Hydrotreating process combines advanced process technology, high-performance catalyst systems and efficient reactor internal designs. Hydrotreating process control is done in the present work by modeling a hydrotreating reactor with Quenching Hydrogen gas. Due to the exothermic reaction of HDT the reactor temperature can increase beyond the design intent, and this is why a good temperature control system is required. The reactor should have a temperature control single loop to control and monitor pressure and temperature rise inside the reactor, this was mainly done by the inlet quenching hydrogen gas to the reactor. [1]

The reaction temperature is a process variable that affects the conversion degree of the reactants, selectivity, and catalyst regeneration. High reactor temperatures improve HDT reaction rates but may cause more hydrocracking of the feed, decrease the desired product yield and increase gas production. Also, high temperatures enhance coke formation and decay catalyst cycle life. Since performing the desired conversion can be limited by temperature increase, the total catalyst volume is frequently separated into several beds divided by the inter bed zones for introducing quench fluids. Crud-e oil fractions, particularly highly unsaturated fractions, are known for being H₂-required feeds during hydrotreating. Processing of these feeds generates huge amounts of heat during HDT process, which can lead to a sharp temperature increase along the reactor. H₂ quenching has been the most famous way to control temperature in most HDT processes. [1]- [2]

2. Materials and Methods

2.1 Materials

Operating and control philosophy for main equipment and main process are as follows.

The use of the reactor model is exemplified in a Fixed Bed reactor with a NiMo commercial catalyst (300 m²/g specific surface area, 0.56 cm³/g pore volume, 127Å mean pore diameter, 0.8163 g/cm³ bulk density, 10.7 wt% Mo, 2.9 wt% Ni) and Visbroken diesel (37°API, 573mg/kg sulfur, 236ppm total nitrogen, 518 wppm basic nitrogen, 12.6 vol% total aromatics, 160 to 340°C distillation range) as hydrotreating feed.

The following reaction conditions were used: pressure of 108 kg/cm², H₂/oil ratio of 500Sft³/bbl, LHSV of 2.5 h⁻¹, and a reaction temperature is 340°C is for steady state model. [1]

Table 1: The reactor conditions

Item	Value
F	Volumetric feed rate ,0.00273m ³ /s
V	reactor volume , 40m ³
C _{A0}	Concentration of Aromatic in feed, 0.43 mol/L
k _{of}	Pre exponential factor for forward reaction 1.041 × 10 ⁵
K _{or}	pre exponential factor for reverse reaction. 8.805×10 ⁹
E	Activation Energy,121400j/mol for forward reaction, 186400 j/mole for reverse reaction
PH	pressure of hydrogen gas 108 kg/m ²
R	Gas constant 8.314 j/mol.k
ΔH	Heat of reaction -255000 j/mol
ρ	Fluid density, 832.1 kg/m ³
C _p	Fluid heat capacity 2000j/kg K
T ₀	673k
T	650k
T _q	357k
T _s	823k
C _{As}	0.22 mol/L
A	30m ²

2.2 Methodology

Process modeling began by determination of mass and energy balance from the general moles balance. First the system must be linearized about the steady state point. As model statement define that only diesel feed temperature (T) and hydrogen quenching temperature (T_q) changes during HDT [1]. A Taylor series for these variables about the steady state point for energy balance is performed to define the deviation variables at the steady state point. Then the steady state equations are subtracted from the unsteady state equation and deviation variable is substituted.

The system can be rewritten with constants for the partial derivatives as ODE, after that the Laplace transforms for this system can be taken and the transfer function is determined. After determining the transfer function it is important to know if the system is stable or not, this is performed by defining the open loop characteristic equation. If any roots of its characteristic equation lie in the right hand side of the imaginary axis, the system will be unstable otherwise the system is stable.

If the system is unstable then many options of controller to operate the hydrotreating unit is available. For example we can use proportional controller or proportional plus derivatives controller or proportional integral derivative controller.

Later the overall transfer function was defined, the characteristic equation is taken and by adopting Routh array elements of first column are selected to get the value of controller parameters (K, K_i and K_{td}). These value of controller parameters make the response of the controlled variable remain stable.

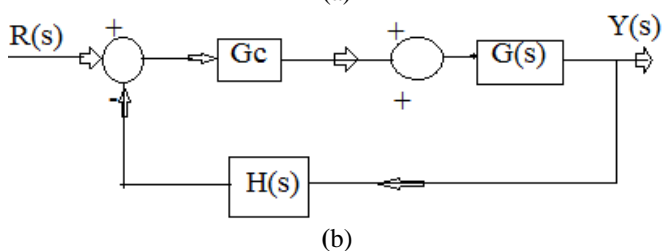
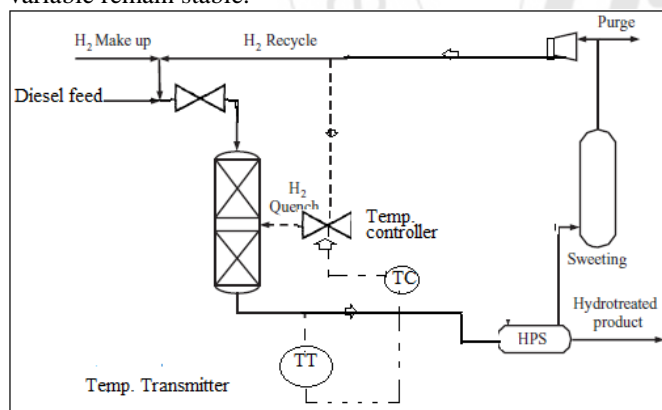


Figure 2: (a) A single control loop of the reactor temperature.

(b) The Block diagram of temperature control loop. Where G_c is a controller or compensator is, G_s represents the

process model, and H(s) represents the measurement dynamics. Y(s) represents the controlled variable, R(s) represents the reference input.

3. Results & Discussion

3.1 Modeling of Process Dynamic

Description of reactor model in previous sections is taken as a base for developing the dynamic heterogeneous one dimensional reactor model. This model is based on the two film theory and makes use of correlations to estimate heat and mass balance.

4.1.1 Model Equations

4.1.1.1 General moles balance equation

Accumulation = Moles in – Moles out + Moles generated (1)

$$\frac{dn_A}{dt} = n_A(in) - n_A(out) + rv \quad (2)$$

Where

n_A ~ Number of moles for aromatic compounds

r ~ Rate of the reaction

v ~ Volume of the reactor

But

$$n_A = F \times C_A \quad (3)$$

Where

F ~ mole flow rate of diesel fluid

C_A ~ Aromatic concentration in the fluid

So equation (3) will be

$$v \frac{dC_A}{dt} = FC_{A_o} - FC_A + rv \quad (4)$$

Divide eq. (4) by V

$$\frac{dC_A}{dt} = \frac{F}{V} (C_{A_o} - C_A) + r \quad (5)$$

From the literature the rate of the reaction for hydrogenation of aromatics is equal

$$r_{HDA} = k_f p_{H_2}^G C_A^S - k_r (1 - C_A^S) \quad (6)$$

Substitute (6) in (5)

$$\frac{dC_A}{dt} = \frac{F}{V} (C_{A_o} - C_A) + k_f p_{H_2}^G C_A^S - k_r (1 - C_A^S) \quad (7)$$

The Rate constant is

$$K = k_o e^{\frac{-E}{RT}} \quad (8)$$

Substitute (8) in (7)

$$\frac{dC_A}{dt} = \frac{F}{V} (C_{A_o} - C_A) + k_{of} e^{\frac{-E}{RT}} p_{H_2}^G C_A^S - k_{or} e^{\frac{-E}{RT}} (1 - C_A^S) \quad (9)$$

Equation number 4.15 represent the material balance equation

$$\frac{dy_1}{dt} = \frac{\partial f_1}{\partial T_s} y_1 + \frac{\partial f_1}{\partial T_{Qs}} y_2 \quad (19)$$

4.1.1.2 Energy balance

Heat Accumulated = Heat in – Heat out + heat Generated – Q quench (10)

$$y_1(0) = y_2(0) = 0 \quad (20)$$

The system can be rewritten with constants for partial derivatives as follow

Q quench is the amount that heat transfer to the hydrogen gas which equal to

$$\frac{dy_1}{dt} = a y_1 + b y_2 \quad (21)$$

$$V\rho c_p \frac{dT}{dt} = mc_p(T_0 - T) + rv\Delta H - Q \quad (11)$$

Taken Laplace transforms of this system

But $Q = (UA)(T - T_Q)$ (12)

$$sY_1(s) = aY_1(s) + bY_2(s) \quad (22)$$

Eq. (12) is applied in in Eq. (11) and Divided by $v\rho c_p$

Now transfer function must be obtain by solving the system

$$\frac{dT}{dt} = \frac{F}{V}(T_0 - T) + \frac{r}{\rho c_p} \Delta H - \left(\frac{UA}{v\rho c_p} \right) (T - T_Q) \quad (13)$$

$$(s - a)Y_1(s) = bY_2(s) \quad (23)$$

$$G_s = \frac{Y_1}{Y_2} = \frac{b}{(s - a)} \quad (24)$$

Eq.(8) is substituted in eq.(13)

Now the value of a and b coefficient are obtained from the partial derivatives.

$$\frac{dT}{dt} = \frac{F}{V}(T_0 - T) + \frac{\left(k_{of} e^{\frac{-E}{RT}} p_{H_2}^G C_A^S - k_{or} e^{\frac{-E}{RT}} \right) \times \Delta H}{\rho c_p} - \left(\frac{UA}{v\rho c_p} \right) (T - T_Q) \quad (14)$$

$$a = \left(\frac{\partial f_1}{\partial T_q} \right)_s = \frac{\left[\frac{F}{V}(T_0 - T) + \frac{\left(k_{of} e^{\frac{-E}{RT}} p_{H_2}^G C_A^S - k_{or} e^{\frac{-E}{RT}} \right) \times \Delta H}{\rho c_p} - \left(\frac{UA}{v\rho c_p} \right) (T - T_Q) \right]}{\partial T_q} \quad (25)$$

Equation number 14 is the energy balance equation

First, the system was linearized about the steady-state point, then Laplace transforms was taken to yield the final transfer function .Due to the exothermic reaction the temperature and concentration change with time.

The Taylor series for these variables (T, T_Q) about the steady state point for the energy balance is

$$a = \frac{UA}{V\rho c_p} = \frac{30 \times 35}{40 \times 832.1 \times 2000} = 1.5 \times 10^{-5} \quad (26)$$

$$\frac{dT}{dt} = f_1(T, T_Q) = f_1(T_s, T_{Qs}) + \frac{\partial f_1}{\partial T} (T - T_s) + \frac{\partial f_1}{\partial T_Q} (T_Q - T_{Qs}) \quad (15)$$

$$b = \left(\frac{\partial f_1}{\partial T} \right)_s = \frac{\left[\frac{F}{V}(T_0 - T) + \frac{\left(k_{of} e^{\frac{-E}{RT}} p_{H_2}^G C_A^S - k_{or} e^{\frac{-E}{RT}} \right) \times \Delta H}{\rho c_p} - \left(\frac{UA}{v\rho c_p} \right) (T - T_Q) \right]}{\partial T} \quad (27)$$

At the steady state point

$$\frac{dT_s}{dt} = f_1(T, T_{Qs}) \quad (16)$$

The deviation variables about the steady-state point are defined as

$$Y_2 = T - T_s \quad (17)$$

$$Y_2 = T_Q - T_{Qs} \quad (18)$$

When the steady state equation are subtract from the unsteady state equation and deviation variable is substituted the balance become.

$$b = -\frac{F}{V} + \left(\frac{-\Delta H}{\rho c_p} \right) \left[\left(\frac{E}{RT_s^2} \right) K_{0f} e^{\frac{-E}{RT}} PHC_{AS} - \left(\frac{E}{RT_s^2} \right) K_{0r} e^{\frac{-E}{RT}} C_{AS} - \left(\frac{UA}{v\rho c_p} \right) \right] \quad (28)$$

Substitute all the items value from table 1 in eq. (27)

$$b = \frac{0.00273}{40} + \left(\frac{255000}{832.1 \times 2000} \right) \times \left[\left(\frac{121400}{8314.5 \times 823^2} \right) \times 1.041 \times 10^5 \times e^{\frac{-121400}{8314.5 \times 823}} \times 0.47 - \left(\frac{186400}{8314.5 \times 823^2} \right) \left(8.805 \times 10^9 \times e^{\frac{-186400}{8314.5 \times 823}} \right) + \left(\frac{186400}{8314.5 \times 823^2} \right) \times \left(e^{\frac{-186400}{8314.5 \times 823}} \right) \times 0.47 \right] - 1.5 \times 10^{-5} \quad (29)$$

$$b = -43438.27 \text{ s}$$

But

$$G_s = \frac{Y_1}{Y_2} = \frac{b}{(s-a)}$$

The T.F is then

$$G_s = \frac{Y_1}{Y_2} = \frac{-43438.27}{s - 1.5 \times 10^{-5}}$$

The open loop characteristic equation is the dominator of the T.F

$$s - 1.5 \times 10^{-5} = 0$$

So the root of the open loop T.F is

$$s = 1.5 \times 10^{-5}$$

4.2 Hydrotreating Process Control

Since the value of the root is positive real number the system is unstable. It is proposed to use a proportional plus derivative controller. The controller will be used to manipulate the quenching hydrogen temperature to control the reactor temperature. From Process control diagram in Figure 2

The open-loop transfer function is $G_c G(s) H(s)$

The closed loop transfer function is

$$\frac{C(s)}{R(s)} = \frac{G_c G_s}{1 + G_c G_s} \quad (30)$$

The proportional pulse derivatives controller equation is

$$G_c(s) = K(1 + T_D S) \quad (31)$$

Substitute eq. (24) and (31) in (30)

$$\frac{C(s)}{R(s)} = \frac{K(1 + T_D S) \times \frac{a_{22}}{(s - b_{21})}}{1 + K(1 + T_D S) \times \frac{a_{22}}{(s - b_{21})}} \quad (31)$$

$$\frac{C(s)}{R(s)} = \frac{K(1 + T_D S) \times \frac{-43438.27}{(s - 1.5 \times 10^{-5})}}{1 + K(1 + T_D S) \times \frac{-43438.27}{(s - 1.5 \times 10^{-5})}} \quad (32)$$

The closed loop characteristic equation is

$$1 + \text{open loop T.F} = 0$$

$$1 + G_c \times G_s = 0 \quad (33)$$

$$1 + \frac{[K(1 + T_D)S] \times -43438.27}{(S - 1.5 \times 10^{-5})} = 0 \quad (34)$$

$$S - 1.5 \times 10^{-5} - 43438.27K - 43438.27KT_D S = 0$$

Rearrange

$$(1 - 43438.27T_D K)S + [-1.5 \times 10^{-5} - (43438.27K)] = 0 \quad (35)$$

Roth Array for this system

$(1 - 43438.27T_D K)$	0
$-1.5 \times 10^{-5} - 43438.27K$	0

All element in the first column must be positive for stability

$$(1 - 43438.27KT_D) > 0 \quad (36)$$

$$KT_D > 2.3 \times 10^{-5} \quad (37)$$

The second element will be positive if

$$(-1.5 \times 10^{-5} - 43438.27K) > 0 \quad (38)$$

$$K > 3.45 \times 10^{-10} \quad (39)$$

The system is stable for all value all

$$KT_D > 2.3 \times 10^{-5} \text{ m}^3 \cdot \text{K} \cdot \text{S} / \text{mol} \quad \text{and}$$

$$K > 3.45 \times 10^{-10} \text{ m}^3 \cdot \text{K} \cdot \text{S} / \text{mol}$$

4. Discussion

The modelling and control of diesel hydrotreating unit begun by determination of the mole and energy balance equations. From the energy balance the deferential equation for the system was obtained and it was found that it is nonlinear differential equation, then the system was linearized about the steady-state point by using Taylor series for the two

variables (T_Q, C_A), after that the Laplace transforms was taken to yield the process transfer function .

The open loop transfer function was obtained by solving the system and it was found that the system is first order. From the transfer function the open loop characteristic equation was obtained, then the value of the root was calculated and it was found that it is positive real number. Since the value of the root is positive real number the system is unstable (The system will be stable if the root of the characteristic equation lie in the left hand side of the imaginary axis).

It was proposed to use a proportional plus derivative controller. The controller will be used to manipulate the quenching temperature to control the reactor temperature. The closed loop transfer function and the characteristic equation were obtained, then Roth Array was used to obtain the controller parameters (K and KT_D) which make the system stable

5. Conclusions

Process modeling and control can help in better design, optimize and operate the refinery units. Refinery unit is never ever truly at steady state modeling. The transient behavior of the process system is best studied using a dynamic simulation tool like mathematical modelling. With mathematical modelling we can control the process and we will avoid the hazard and operability problems. In process modelling, the dynamic analysis of a process system can provide insight into the process system when it is not possible with blind method such as trial and error or Zeiglar-Nichols.

References

- [1] J. Ancheyta, Modelling and Simulation of Catalytic Reactors for Petroleum Refining, John Wiley & Sons, Inc., Hoboken, New Jersey, 2011.
- [2] H. James, E. Glenn, Petroleum Refining Technology and Economics, Fourth edition, Marcel Dekker publisher, 2001.
- [3] W. Nelson, Petroleum Refinery Engineering, Fourth edition, McGraw-Hill Book Co., New York, 1987.
- [4] M. Fahim, T. Alsahhaf, A. Elkilani, Fundamentals of Petroleum Refining, The Boulevard, UK, 2010.
- [5] P. Paraskevopoulos, Modern Control Engineering, Marcel Dekker, New York, 2002.
- [6] C. Cabrera, Process Refining Handbook, R. A. Myers, Ed., Sections 6.18–6.25, McGraw-Hill Book Co., New York, 1987.
- [7] W. Gruse, D. Stevens, Chemical Technology of Petroleum , 3rd Ed., McGraw-Hill Book Company, New York, pp. 117–121, 306–309, 1960.
- [8] D. Hougau and M. Watson, Industrial Chemical Calculations, John Wiley and Sons, New York, 1938.
- [9] Hengstebeck, R. J. (1959), Petroleum Processing, McGraw-Hill Book Company, New York, pp. 272–279.

Author Profile

Zeyad M.Ahmed received B.S. in Chemistry from university of Khartoum, in 2005. and he received M.S. in petroleum and Petrochemical Technology. From 2005 to 2007 he worked as a part timer teaching assistant at university of Khartoum, faculties of science and engineering department of chemical engineering. In 2008 he worked at petroenergy e and P Company (CNPC Sudan branch) as lab analyst until 2016. From 2016 till now he was working as lecturer at Jazan University.