Development of Intelligent Supervisory Technique for Temperature Profile of A Chemical Reactor by Using Neural Networks and A Physical Model

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ABSTRACT: In VGO hydro-desulfurizing reactor reactor in oil refinery plant, if catalyst at a spot reacts excessively in the reactor, temperature at the spot becomes higher than in the surrounding area. The excessive reaction shortens the lifetime of the catalyst. Therefore the operator monitors temperatures measured at multiple points in the reactor to find abnormally large values in the temperature profile. All process variables of temperatures in the reactor are displayed on control panels, but exact locations of the sensor cannot be shown on the panel because of difficulty in projecting 3D spatial data onto 2D panel. The operator is forced to remember the location of the each measurement point when he watches these variables. In this study, an intelligent supervisory system was developed which calculates temperature profile in the reactor by using online neural networks and plots 3D temperature profile at various height of the reactor. Moreover, the system can estimate temperatures at various location based on a physical model which takes account of one dimensional flow and reaction of two materials.

KEYWORDS: Neural network, Physical model, Supervisory system, Hot spot, VGO hydro-desulfurizing, Chemical process, Temperature profile

INTRODUCTION

In chemical plants, plant operators monitor a great number of process variables simultaneously, in order to find any symptoms which lead the process to a fatal fault. Real time values of process variables are shown to the operator on the CRT screen of Distributed Control System (DCS), and then almost all of them are displayed without any modification. Because of this, the operator has to always check the behavior of closely related variables and based on his heuristic knowledge of the operation, he has to judge whether the relationship between the process variables is normal or not.

In a chemical reactor, state variables such as temperature, concentration and viscosity, are distributed spatially over the reactor vessel. If such a state variable is important to control the reactor, it is usually measured at multiple locations in the reactor. All measured data are displayed on control panels, but exact locations of the sensor cannot be shown on the panel because of difficulty in projecting 3D spatial data onto 2D panel. The operator is forced to remember the location of the each measurement point when he watches these variables. If spatial profile of the variable in the reactor is presented to the operator in real time, operator's load of process monitoring will be reduced because an operator does not have to remember sensor location in order to grasp the state of the reactor.

Moreover, presentation of a reference value that is estimated from the current feed condition of the reactor is helpful to the operator for judging whether the process is normal or not.

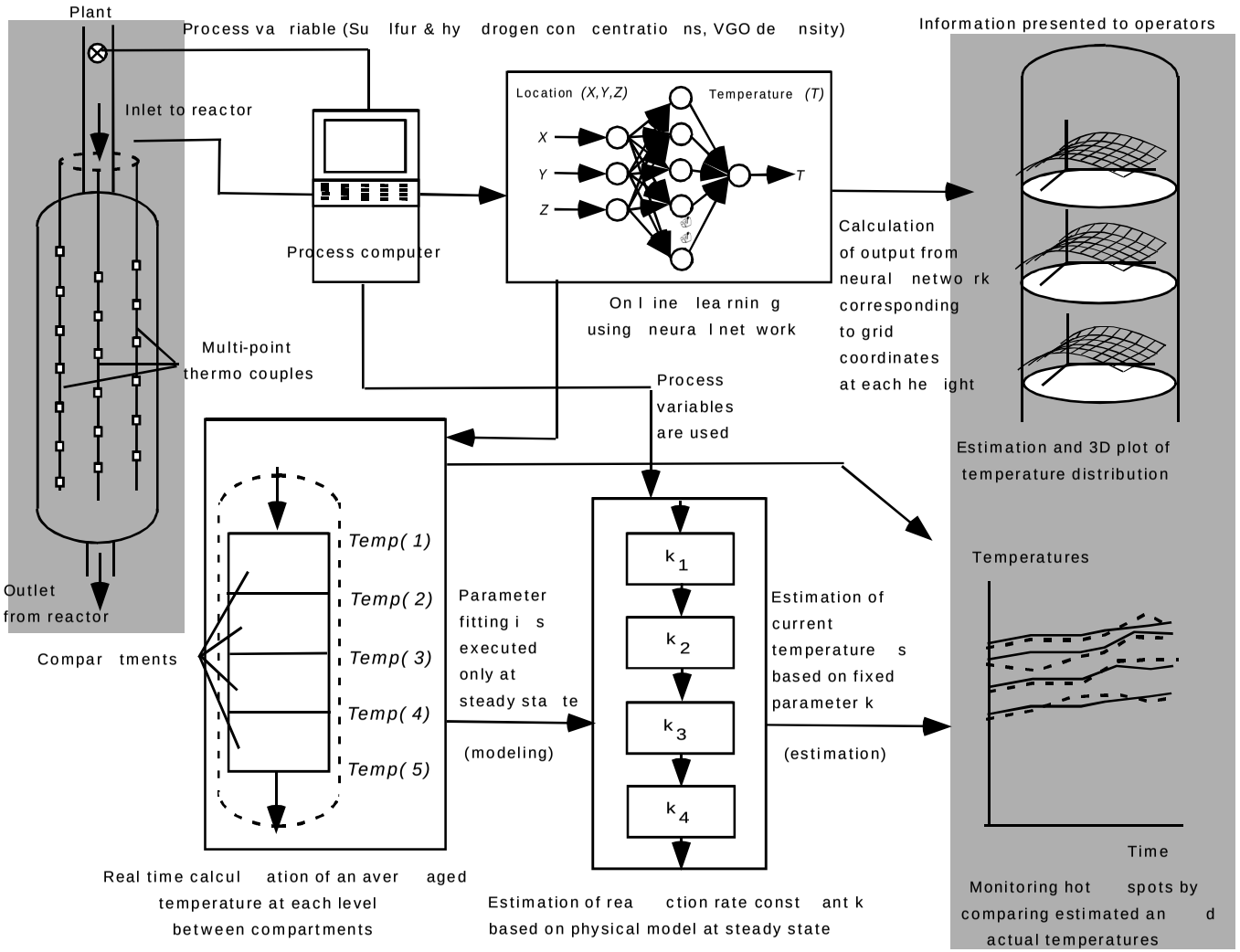

Figure 1: Outline of developed intelligent supervisory system to estimate temperature profiles in order to detect hot spots in VGO hydro-desulfurizing reactor.

In this study, we tackled the problem of detecting hot spots in a VGO hydro-desulfurizing reactor of an oil refinery plant. A system is developed which calculates temperature profile in the reactor by using online neural networks and plots 3D temperature profile at various height of the reactor. Moreover, the system can estimate temperatures at various location based on a physical model which takes account of one dimensional flow and reaction of two materials. In this paper, outline of the system is shown firstly, and neural networks and the details of the physical model are described.

HOT SPOT PROBLEM IN VGO HYDRO-DESULFERIZING REACTOR

De-sulfurization of VGO (Vacuum Gas Oil) is one of the major processes in oil refinery plant. (Nelson 1985, Sekiyu Gakkai 1984) By adding hydrogen into VGO under existence of catalyst, the sulfur atom in the oil is combined with hydrogen and it is removed from the oil as hydrogen sulfur gas. The tower reactor is packed with catalyst and the mixture of VGO and hydrogen gas is fed to the top of the reactor. The oil flows down through vacant space between the catalyst particles and then the reaction occurs on the surface of the catalyst. If catalyst at a spot reacts excessively in this reactor, temperature at the spot becomes higher than in the surrounding area. The excessive reaction shortens the lifetime of the catalyst. Therefore the operator monitors temperatures measured at multiple points in the reactor to find abnormally large values in the temperature profile. Therefore the operator monitors temperatures measured at multiple points in the reactor to find abnormally large values in the temperature profile.
To monitor temperatures in the reactor, three rods of multiple thermocouple, each of which is a long rod attached with several sensors along it, are installed in the reactor (Fig.1). The location of each sensor is arranged so that all measurement points are aligned on a spiral curve from top to bottom in the reactor. Measured data of temperature and other process variables are stored in a process computer. Among many measurable variables, sulfur concentration, hydrogen concentration and VGO density are used in our developed system.

OUTLINE OF THE MONITORING SYSTEM

The system has two main functions: one is calculation of temperature profile, and the other is estimation of temperature using physical model. (Fig.1)
For calculation of temperature profile, a neural network is used to interpolate the temperature data. This calculation is executed at a short interval, and 3D contour of temperature profile at each height is presented to the operator through CRT screen of the process computer. Moreover, averaged temperatures at any height can be calculated as well.
The estimation of temperature consists of two phases: modelling phase and estimation phase. In the modelling phase, the reactor is divided into 4 compartments and reaction rate constant k in each compartment is calculated using averaged temperatures. This calculation is executed when the reactor is at a steady state. In the estimation phase, an expected value of temperature is calculated using estimated k values. This calculation is executed in real time and the result is shown to the operator.

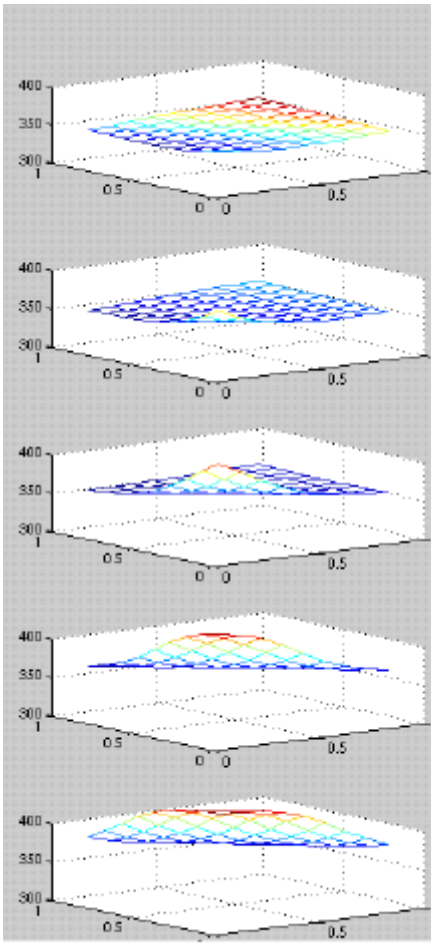

Figure 2: Temperature profile at 5 height when hot spot occurred at (0.26, 0.32, 0.68)

TEMPERATURE INTERPOLATION BY NEURAL NETOWRKS

A three layered back propagation neural network (Rumelhart 1986) is used for interpolation of measurement temperatures. In order to relate the temperature with the location in the reactor, the location coordinate (X, Y, Z) is used as input vector to the neural network, and the measured temperature is used as teaching data. The number of nodes in the hidden layer is fixed to 8. The neural network is trained iteratively over 100,000 times using the learning data. Temperature profile at each height can be obtained by calculating the

temperature at every grid coordinates (X,Y) at height Z using the neutral network. The averaged temperature at each height is calculated from the temperature profile. Fig.2 shows an example of temperature profile when a hot spot occurred actually. The temperature profile at different normalized heights (0.2, 0.35, 0.5, 0.65, 0.8), and a hot spot appeared at (0.26, 0.32, 0.68), which is close to the fourth profile from the top. Hot spot can be easily identified from the 3D figures.

TEMPERATURE ESTIMATION BASED ON PHYSICAL MODEL

Interpolated temperature is essentially different from actual temperature in the reactor. Especially, if a hot spot unfortunately exists at the centre of measurement points, it is difficult to find the hot spot with an approach using temperature interpolation. In such a case, information of other process variables and thermodynamic properties of substances are necessary to make more accurate detection of excess reaction.
The progress of the chemical reaction is calculated by reaction rates; e.g. reaction rate constant becomes larger if excessive reaction occurs. However, it is difficult to obtain an accurate reaction rate constant which is applicable to the actual plant. This is because properties of VGO changes according to the kind of crude oil, and the activity of the catalyst changes with time. From these reasons, the reaction rate constant k should be identified when the reactor is at a steady state. For the period in which it can be assumed that the reactor is steady state, fault in the reactor can be found by comparing the current temperature and temperature calculated based on the obtained k and the physical model.
In order to identify the location of the fault, the reactor is described using a simple compartment model, with one dimensional flow. The reaction rate constant k is calculated for each compartment. The number of compartments is determined to be 4 in this study.

The following assumptions are used when deriving the simple physical model:
1) All sulfur compounds are substituted for thiol (mercaptan) type compounds, each of which has one sulfur atom. (R-SH type) .
2) The material and energy balance equations are derived by assuming that the reactor is steady state.
3) Reaction is written in the form: R-SH + H_2 R-H + H_2S
4) Temperature of material, concentrations of sulfur compounds and hydrogen can be measured on line.

Basic material balance equation is described as

$$(1) \qquad \frac{\partial}{\partial t}([R-SH]rsdx) = -\frac{\partial}{\partial x}([R-SH]rv)sdx - k[R-SH][H_2]rsdx$$

where, [ ] is concentration, x is the distance measured from the top to the bottom, r is density, s is cross sectional area of the reactor, and v is velocity of the material. If the density is constant and the reactor is at a steady state, then

$$(2) \qquad v\frac{\partial}{\partial x}[R-SH] = -k[R-SH][H_2]$$

If initial values of [R-SH], and [H_2] are assumed to be a and b

$$(3) \qquad \begin{cases} [R-SH]_0 = a \\ [H_2]_0 = b \end{cases}$$

Because mole concentration of R-H, H_2S are equal. [H_2] is described as

$$(4) \qquad [H_2] = (b-a) + [R-SH]$$

By substituting for [R-SH],

$$(5) \qquad v\frac{dy}{dx} = -ky\{(b-a)+y\} \quad 0 \le x \le L$$

where L is vertical length of compartment.
From Eq.(5), [R-SH] can be calculated as follows.

$$(6) \qquad y(x) = \frac{b-a}{\left(\frac{b}{a}\right)\exp\{(b-a)kx/v\} - 1}$$

Basic energy balance equation is described as

$$(7) \qquad \frac{\partial}{\partial x}v(m \cdot C)q = -Hv\frac{\partial}{\partial x}[R-SH] - Loss(x) = Hvk[R-SH][H_2] - Loss(x)$$

where q , C, H and Loss(x) are temperature, specific heat, reaction heat, and Loss(x) is heat loss.

$$(8)\quad [R-SH]=y$$
$$[R-H]=a-y+[R-H]_0$$
$$[H_2S]=a-y+[H_2S]_0$$
$$[H_2]=(b-a)+y$$

where, subscript 0 represents values at x= 0.
The left hand side of Eq.(7) can be simplified as follows..

$$(9)\quad v\frac{d(m\cdot C)}{dx}q = v\frac{d}{dx}\{yC_{RSH}+[R-SH]C_{RH}+[H_2S]C_{H2S}+[H_2]C_{H2}\}q$$
$$= v\frac{d}{dx}\{(C_{RSH}-C_{RH}-C_{H2S}+C_{H2})y+((a+[R-H]_0)C_{RH}+(a+[H_2S]_0)C_{H2S}+(b-a)C_{H2})\}q$$
$$\equiv v\frac{d}{dx}(ay+b)q = vaq\frac{dy}{dx}+v(ay+b)\frac{dq}{dx}$$

The right hand side of term of Eq.(7) can be written as

$$(10)\quad -Hv\frac{d}{dx}[R-SH]-Loss(x)=-Hv\frac{dy}{dx}-Loss(x)$$

From Eqs.(7) and (8), the energy balance equation is described as

$$(11)\quad vaq\frac{dy}{dx}+v(ay+b)\frac{dq}{dx}=-Hv\frac{dy}{dx}-Loss(x)$$

If Loss(x) is assumed to be 0, then, as a result, Eq.(12) is obtained.

$$(12)\quad q=q_0 j+(j-1)\frac{H}{a} \qquad \left(j=\frac{aa+b}{ay+b}\right)$$

By the following procedure the reaction rate constants can be calculated from material and energy balances.
1) Measure process variables (sulfur and hydrogen concentration, temperature and flow velocity of the material) at a steady state.
2) Calculate averaged temperature at top and bottom of compartments are calculated by using neural network.
3) Calculate the sulfur concentration at x=L, using Eq.(12), and the averaged temperature.
4) Calculate the reactor rate constant k, is from Eq.(6).
5) In the estimation phase, using k values obtained in 4), the temperature at bottom of each compartment is calculated and the result compared with actual temperature measurement.
We referred to a data book on material property (API 1983) for specific heat and reaction heat of the substances.

Fig.3 shows an interface panel of the hot spots monitoring system. Upper figures show trend of 3D temperature profile. A new profile calculated at the next time is drawn on the right hand of the current window and this procedure circulates. The bottom figures shows the reaction rate constant, temperature, concentrations of materials and reactants, and de-sulfurized ratio .This figure shows that new reaction rate constants have just calculated from temperatures,. As the result of parameter fitting, the estimated concentration at each boundary becomes a little different from old one. The concentration curve along the height of the reactor can be monitored also. Desulfured ratio means the sulfur concentration at the bottom is divided by that at the top. This index shows the overall activity of the catalyst in the reactor.
This system was installed in the control system of the VGO hydro-desulfurizing reactor. The operator is tuning and testing the monitoring system. They say this system is also applicable to estimate the allowance of set point change of temperature and useful to know if catalyst could be packed heterogeneously.

CONCLUSION

In this study, a system was developed which calculates temperature profile in the reactor by using online neural networks and plots 3D temperature profile at various height of the reactor. Moreover, the system can estimate temperatures at various location based on a physical model which takes account of one dimensional flow and reaction of two materials.

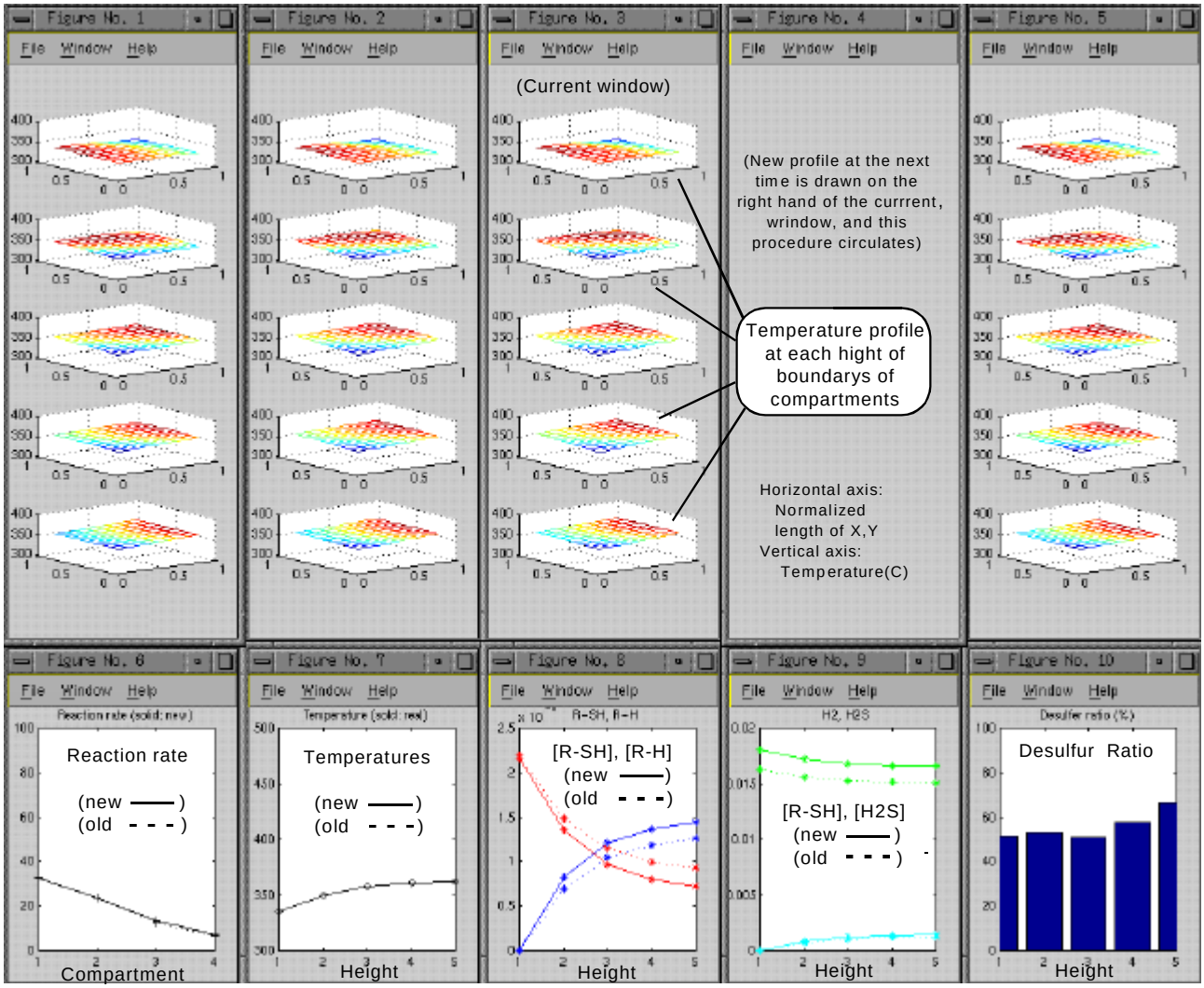

Figure 3: An interface panel of the hot spots monitoring system of VGO hydro-desulfurizing reactor (Upper side: trend of temperature profiles at each height, Lower side: reaction rate constant, temperature, concentration of substance, and desulfur ratio)

Averaged temperature can be calculated because of interpolating measured temperature by neural network, moreover first dimensional physical model can be used. As the result, not only temperature, but also estimated values of reaction rate constant, concentration of materials and reactants can be presented to the operator.
In actual plant, simple and adaptive model is more effective than theoretical detailed model. Combination of neural network and simple physical model can be adapted for the changes of crude oils and deterioration of catalyst.
This system is used by the operator in a actual plant to evaluate it. In future works, the evaluation of the monitoring system in the actual plant should be studied.

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