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Application of a Model-based Fault Detection and Diagnosis System to a Hydrotreating Reactor

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This work presents the development of a quantitative model-based fault detection and diagnosis (FDD) applied to a simulated diesel fuel hydrotreating (HDT) unit. The proposed FDD algorithm classifies the discrepancies (expressed as residuals) between the actual system behavior − represented by a phenomenological model − and that of the system model, using a geometric distance technique. Laguerre functions, with variable parameters given by interpolated lookup table values, were chosen as the system model. Disturbances in input variables of the 1st hydrogenation reactor were assumed and the HDT unit was simulated in order to generate cases representing normal and abnormal (disturbed) operational conditions. Examples are shown in which the FDD system was able to correctly classify the studied cases, using data from a time window of 30 min.

1. Introduction

Fault detection and diagnosis FDD is an area of process control that has been subject to a considerable growth in the last years. A fault is a departure of at least one characteristic property or variable of the system from an acceptable range and may occur in the process, controller, sensors and/or actuators (Chiang *et al.*, 2001; Venkatasubramanian *et al.*, 2003). The early detection and diagnosis of faults may help process personnel to confidently operate their plant installations.

The hydrotreating (HDT) process used in modern refineries to catalytically desulfurize oils may be particularly benefited from the application of FDD techniques, as it is an exothermic process operated under several safety constraints. Accidents in HDT units may be devastating and costly (Ancheyta and Speight, 2007). Additionally, this process is very important because of global clean-fuel regulations.

Quantitative or qualitative FDD techniques may be developed using model or history-based knowledge (Venkatasubramanian *et al.*, 2003). Here, a quantitative model-based FDD approach is developed and applied to a simulated HDT process subject to changes in the feed concentration of sulfur. The proposed approach uses Laguerre functions as input-output models in order to generate residuals with the actual (simulated) system behavior. The residuals are classified using geometric classification based on Euclidean distance (Isermann, 2005). Results of detection of abnormal operation are shown using the simulation of a phenomenological model (Carneiro, 1992).

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2. Fundamentals

2.1 HDT Unit Description and Phenomenological Model

An HDT plant is composed by a reaction section – which includes a series of pre-heating furnaces, the reactors, the hydrogen flash system and the make-up compressor for hydrogen – and a stabilization section. Usually, two reactors are employed. The reactors are trickle bed ones as the inflow enters in gaseous and liquid phases, composing a triphasic system together with hydrogen and the catalyst solid bed. A quench system is used to control the temperature of the reactors. This is achieved with the injection of a H_2 flow in the middle of catalytic beds. The yield products of this unit are directed to stabilization section, where all commercial specifications are adjusted.

An HDT model developed by Carneiro (1992) was used here. The model shows a similar dynamic to existing Brazilian units (Carneiro, 1992). Each reactor comprises two beds in series. The assumptions of the model for the reactor were:

- Only one reaction occurs and this reaction is 1st order with respect to the average concentration of a unique pseudo-reactant A in the pores of the solid phase;
- There is only one fluid phase, with constant physical-chemical properties;
- There is only one solid phase;
- There are no transversal transport phenomena, only longitudinal;
- There is no phase equilibrium;
- The reaction rate is described by the Arrhenius equation;
- There is no variation of volume in the reaction;
- Non-linear interactions between thermal and kinetic processes exist.

The model of the reactor was built assuming that the reactor is composed by 12 CSTR-cells (or stages) in series. The fluid phase flows from the left to the right, but back mixtures (in the reverse direction) also happen between successive stages.

The mass balance for compound A in fluid phase at stage i can now be written:

$$\{V_Z(1+K_m)C_{i-1}+V_Z.K_m.C_{i+1}\}-\{(2K_m+1)V_Z.C_i+K_g.a.V(C_i-C_{i_S})\}=\left\{\nu V\frac{dC_i}{dt}\right\} \quad (1)$$

where: V_Z is the volumetric flow; K_m is an adimensional constant; K_g, the mass transport coefficient; a, the external surface area of solid catalyst particles per total stage volume; V, the total stage volume; ν is the interparticle porosity; C_{i-1}, the concentration of reactant A in fluid phase in previous stage; C_{i+1}, the concentration in next stage; C_i, the concentration in stage i; C_{is} is the concentration in the inner catalyst pore.

The mass balance in solid region at stage i is given by:

$$\{K_g.a.V(C_i-C_{i_S})\}=\left\{V(1-\nu)\frac{dC_{i_S}}{dt}\right\}+\left\{V(1-\nu)k_0.C_{i_S}.e^{\frac{E}{(R.T_{i_S})}}\right\} \quad (2)$$

where: k_0 is the Arrhenius kinetic constant; E, the activation energy; R, the universal gas constant and T_{iS}, the absolute solid temperature.

The energy balance in fluid phase at stage i is described by:

$$\left\{V_Z(1+K_h)\rho.C_P.T_{e_{i-1}} + V_Z.K_h.\rho.C_P.T_{e_{i-1}} + U.a.V\left(T_{e_{iS}} - T_{e_i}\right)\right\} - \left\{(2K_h+1)V_Z.\rho.C_P.T_{e_i}\right\} = \left\{\nu.V.\rho.C_P.\frac{dT_{e_i}}{dt}\right\} \quad (3)$$

where K_h is an adimensional constant; ρ, the gas specific mass; C_p, the gas specific heat; U, the global heat transfer coefficient between flow phase and catalyst; T_{es}, the fluid temperature in the bed; T_{ei-1}, the fluid temperature in the previous stage; T_{ei+1}, the fluid temperature in the next stage; T_{ei}, the fluid temperature in stage i.
The energy balance in solid region at stage i is presented in the following:

$$\left\{U.a.V\left(T_{e_i} - T_{e_{iS}}\right)\right\} + \left\{(-\Delta H_r)V(1-\nu)k_0.C_{i_S}.e^{\frac{-E}{(R.T_{iS})}}\right\} = \left\{V(1-\nu)\rho_S.C_{P_S}.\frac{dT_{e_{iS}}}{dt}\right\} \quad (4)$$

The furnace was modelled using an empirical equation of energy balance. The mixers located after the beds were modelled with a mass balance, each one generating only one equation. A simulation algorithm was developed to represent the 1st bed of the 1st reactor and was implemented in Simulink™. The parameters were: $(-\Delta H_r)=1.28\ 10^5$ J.mol^{-1}; $k_0 = 7.0\ 10^6$ s^{-1}; $(E / R) = 1.0\ 10^4$ K^{-1}; $K_m = 0$; $K_h = 1$; $U.a = 1.4\ 10^5$ W. K^{-1}. m^{-3}; Kg.a = 5.6 s^{-1}; ρ.Cp = 5.0 10^4 J. K^{-1}. m^{-3}; $\rho_s.Cp_s = 1.25\ 10^6$ J. K^{-1}. m^{-3}; a = 1400 m^{-1}; V= 0.5 m^3; ν = 0.4; A = 0.48 m^2.

2.3 Input-output Laguerre Function Based Models for the FDD Approach
For any p > 0, Laguerre functions are defined as (Lee, 1960):

$$l_i = \sqrt{2p}\frac{e^{pt}}{(i-1)!}\frac{d^{i-1}}{dt^{i-1}}\left(t^{i-1}e^{-2pt}\right) \quad (5)$$

which satisfy the following orthonormal properties:

$$\int_0^\infty l_i^2(t)dt = 1 \quad (6)$$

$$\int_0^\infty l_i(t)l_j(t)dt = 0, \qquad i \neq j \quad (7)$$

According to Wylie (1960), any arbitrary functions f(t) can be expanded into infinite series based on Laguerre functions. Considering the unit impulse response h(t) of an unknown function f(t) as given by $h(t) = c_1\ l_1 + c_2\ l_2 + \ \ldots + c_i\ l_i$, where, according to Lee (1960), $c_i = \int_0^\infty h(t)l_i dt$, applying Laplace transform to h(t), the transfer function G(s) of an unknown system may be written as:

$$G(s) = \sqrt{2p}\left[\frac{c_1}{s+p} + \frac{c_2(s-p)}{(s+p)^2} + \ldots + \frac{c_i(s-p)^{i-1}}{(s+p)^i} + \ldots\right] \quad (8)$$

According to Lee (1960), this series can be truncated after a finite number of terms. The models used in the FDI technique were input-output models based on Laguerre functions. The input variables were feed flowrate and input temperature to the 1st bed of the 1st reactor. The output variable was the output temperature of that bed.

3 - Methodology

The phenomenological model was simulated in order to generate dynamic historical data to estimate the parameters of the input-output model. Considering a defined steady-state condition (feed flowrate: 0,1 m^3/s; input temperature: 215.0 ºC; feed concentration: 22.0 mol/m^3), simultaneous disturbances were applied (feed flowrate: sequential steps of ±0.005 m^3/s up to the limit of ±0.5 m^3/s and analogously to the input temperature: ±0.2°C up to ± 2.0 ºC). The parameter estimation was accomplished using the method of least-squares. The infinite series was truncated after the 3rd term. Due to the nonlinearity of the process, an specific set of parameters of the linear input-output model was obtained for each disturbance condition simulated. So, in order to employ the specific parameters for the corresponding operational conditions, the linear input-output in the FDD algorithm was coupled with a 'Lookup Table' technique and a Lagrange interpolation function.

The normal and abnormal conditions in Table 1 were simulated for the FDD study. For these cases, the input temperature was kept at the steady-state value.

Table 1-Operational Conditions for the Studied Cases

Case	Feed concen-tration (mol/m^3)	Feed flow-rate (m^3/h)	Process condition
1	22	0.1	Normal
2	17	0.1	Normal
3	22	0.07	Normal
4	17	0.07	Normal
5	24.5	0.115	High concentration and flowrate
6	24.5	0.055	High concentration and low flowrate
7	14.5	0.115	Low concentration and high flowrate
8	14.5	0.055	Low concentration and flowrate
9	24.5	0.1	High concentration
10	14.5	0.1	Low concentration
11	22	0.055	Low flowrate
12	22	0.115	High flowrate
13	17	0.055	Low flowrate
14	17	0.115	High flowrate
15	24.5	0.07	High concentration
16	14.5	0.07	Low concentration

White noise (mean: 0; standard-deviation: 1) was added to the simulated output variable in order to mimic a realistic situation. Residuals were generated for the 16 cases by comparing the actual (simulated) process response with that of the input-output model. These residuals defined standard conditions to be used during the FDD procedure.
The FDD algorithm was developed to proceed as follows:

- during the operation of the process, data was collected with a sampling time of 50 s considering time windows of 30 min (36 sampling points);
- using the actual values of the input variables, the input-output model was used to calculate predictions of the output variable and the residual was generated;
- the residual values were compared, point by point, with the standard residuals associated to the 16 operational conditions in Table 1;
- for each point, a geometric classification was applied, so that the nearest case – with the smaller Euclidean distance – in Table 1 was established;
- The winner case was declared as the more frequent one, considering all the (36) sampling points analysed.

4 – Results and Discussion

The proposed FDD algorithm was tested with simulated data corrupted by noise. The results are summarized in Table 2. As can be appreciated in the diagonal of Table 2, the case declared as winner is correct for all the situations analysed.
The input-output model is able to predict the effects in the output temperature of disturbances in the feed flowrate and in the input temperature. So, for cases 1, 3, 11 and 12, the residuals have a zero mean. However, the FDD algorithm is able to successfully distinguish between these four cases by using the measurement of the flowrate which is readily available from the supervisory system. Additionally it should be noticed that the correct case has the highest percentage for each situation analysed.
As the input-output model is unable to predict the effects in the output temperature of disturbances in the input concentration, the residuals have non-zero means, presenting an increasing (for cases 5, 6, 9, 15) or decreasing (for cases 2, 4, 7, 8, 10, 13, 14, 16) trend with time, which is successfully identified by the FDD algorithm.

Table 2 Results for the FDD technique

	Nearest Case															
Case	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**
1	**27.78%**	2.78%	19.44%	2.78%	0.00%	0.00%	0.00%	2.78%	0.00%	0.00%	16.67%	25.00%	2.78%	0.00%	0.00%	0.00%
2	2.78%	**52.78%**	2.78%	16.67%	0.00%	0.00%	0.00%	8.33%	0.00%	2.78%	0.00%	2.78%	2.78%	8.33%	0.00%	0.00%
3	19.44%	0.00%	**30.56%**	0.00%	5.56%	0.00%	0.00%	0.00%	0.00%	2.78%	22.22%	13.89%	0.00%	0.00%	2.78%	2.78%
4	2.78%	11.11%	0.00%	**50.00%**	0.00%	0.00%	13.89%	8.33%	2.78%	0.00%	0.00%	0.00%	11.11%	0.00%	0.00%	0.00%
5	0.00%	0.00%	2.78%	0.00%	**55.56%**	2.78%	0.00%	0.00%	25.00%	0.00%	5.56%	0.00%	2.78%	0.00%	5.56%	0.00%
6	2.78%	0.00%	0.00%	0.00%	8.33%	**55.56%**	0.00%	0.00%	19.44%	0.00%	2.78%	2.78%	0.00%	0.00%	8.33%	0.00%
7	0.00%	5.56%	0.00%	2.78%	0.00%	0.00%	**52.78%**	8.33%	0.00%	16.67%	0.00%	0.00%	8.33%	2.78%	0.00%	2.78%
8	0.00%	5.56%	0.00%	8.33%	0.00%	0.00%	2.78%	**61.11%**	2.78%	0.00%	2.78%	0.00%	2.78%	2.78%	0.00%	11.11%
9	2.78%	0.00%	2.78%	0.00%	16.67%	13.89%	2.78%	2.78%	**41.67%**	0.00%	0.00%	0.00%	0.00%	0.00%	16.67%	0.00%
10	2.78%	0.00%	0.00%	0.00%	0.00%	0.00%	16.67%	8.33%	0.00%	**52.78%**	0.00%	0.00%	5.56%	2.78%	0.00%	11.11%
11	16.67%	0.00%	16.67%	0.00%	0.00%	2.78%	0.00%	0.00%	5.56%	0.00%	**41.67%**	11.11%	0.00%	0.00%	0.00%	5.56%
12	16.67%	5.56%	13.89%	0.00%	5.56%	0.00%	0.00%	2.78%	0.00%	0.00%	22.22%	**33.33%**	0.00%	0.00%	0.00%	0.00%
13	0.00%	5.56%	2.78%	16.67%	2.78%	0.00%	5.56%	2.78%	0.00%	0.00%	2.78%	0.00%	**52.78%**	5.56%	0.00%	2.78%
14	2.78%	13.89%	2.78%	0.00%	0.00%	0.00%	2.78%	13.89%	0.00%	5.56%	0.00%	2.78%	0.00%	**50.00%**	0.00%	5.56%
15	0.00%	0.00%	0.00%	0.00%	8.33%	16.67%	0.00%	0.00%	16.67%	2.78%	2.78%	0.00%	2.78%	0.00%	**50.00%**	0.00%
16	0.00%	2.78%	0.00%	0.00%	0.00%	0.00%	2.78%	11.11%	2.78%	8.33%	0.00%	2.78%	0.00%	5.56%	2.78%	**61.11%**
C	22.0	17.0	22.0	17.0	24.5	24.5	14.5	14.5	24.5	14.5	22.0	22.0	17.0	17.0	24.5	14.5
V	0.100	0.100	0.070	0.070	0.115	0.055	0.115	0.055	0.100	0.100	0.055	0.115	0.055	0.115	0.070	0.070
T	215.0	215.0	215.0	215.0	215.0	215.0	215.0	215.0	215.0	215.0	215.0	215.0	215.0	215.0	215.0	215.0

T – input temperature (ºC), V- feed flowrate (m^3/s) e C – feed concentration (mol/m^3)

An extrapolation test (feed concentration 10 mol/m^3 and the feed flowrate 0.2 m^3/s) was also proceeded. For this 'studied case', the nearest standard case should be case 7, which is effectively the one chosen by the FDD algorithm, albeit with a low percentage (30.56 %), followed by case 10 (19.44 %) as can be appreciated in Figure 1.

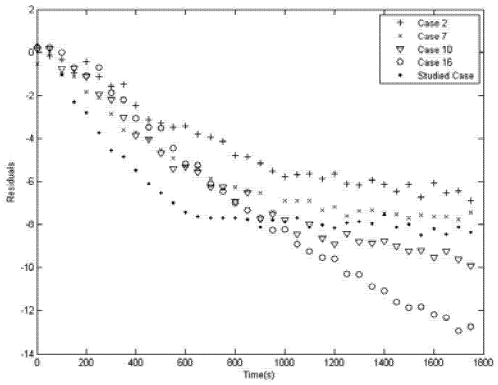

Figure 1 Extrapolation Test for the FDD algorithm

6 - Conclusions

The proposed FDD system correctly classified all the situations investigated, including an extrapolation test. The approach is readily extendable by the inclusion of newer standard conditions. Additionally, the approach of using a input-output model based on Laguerre functions with variable coefficients given by a lookup table coupled with a Lagrange interpolation function proved to be computationally efficient. This support system is expected to help the operator to take confident decisions in the important case of feed concentration disturbances even when this specific measurement is unavailable.

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