GREY-BOX MODELLING OF AN INDUSTRIAL HYDRODESULPHURIZATION PROCESS

E. Gómez [a], C. de Prada [a], D. Sarabia [a], C. A. Méndez [b], S. Cristea [a], J. M. Sola [c], E. Unzueta [c]

[a] Dpt. of Systems Engineering and Automatic Control, Faculty of Sciences, University of Valladolid, Spain

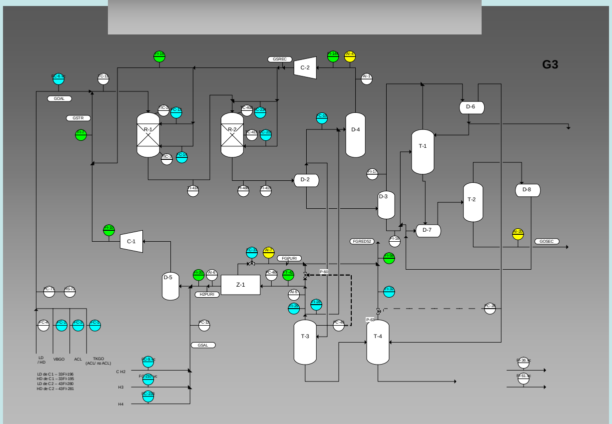
[b] INTEC, Litoral National University – CONICET, Santa Fe, Argentina

[c] Dpt. of Advanced Control, Petronor, Repsol YPF, Muskiz, Bilbao, Spain

Abstract

A reduced order model of a hydrodesulphurization plant which aims to provide dynamic hydrogen consumption rates as a function of the plant hydrocarbon load is being developped. This is part of a wider project oriented to the optimal management of the hydrogen network of a refinery, where hydrogen production should be dynamically adjusted to consumption as much as possible so as to reduce excess losses. The proposed model combines physico-chemical principles with black box elements.

HYDRODESULPHURIZATION UNIT



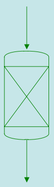
- On-line analyzers
- Simulation boundaries: process manipulated variables (real decision ones); measured
- Redundant variables: measured but not manipulated variables, used in reconciliation

REDUCED DYNAMIC MODEL

COMPONENTS

H_2, CH_4, S, HC (hydrocarbon)

Reactor - dynamic model



$$0 = WM_{IN\_R} - WM_{OUT\_R}$$

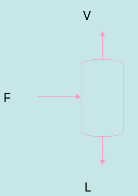
M_L |=| kmol, x |=| %1 mol, WM_i |=| kg/h, W_i |=| kmol/h

$$M_L \cdot x_{H2}^{R}{}' = W_{IN\_R} \cdot x_{H2}^{IN\_R} - W_{OUT\_R} \cdot x_{H2}^{R} - ce_{H2\_S} \cdot k\_r_S \cdot x_{H2}^{R} \cdot x_S^R \cdot M_L - k\_r_{H2} \cdot x_{H2}^{R} \cdot M_L$$

$$M_L \cdot x_S^{R}{}' = W_{IN\_R} \cdot x_S^{IN\_R} - W_{OUT\_R} \cdot x_S^{R} - k\_r_S \cdot x_{H2}^{R} \cdot x_S^R \cdot M_L$$

$$M_L \cdot x_{CH4}^{R}{}' = W_{IN\_R} \cdot x_{CH4}^{IN\_R} - W_{OUT\_R} \cdot x_{CH4}^{R} + k\_r_{lig} \cdot x_{H2}^{R} \cdot M_L$$

Flash drum – static model



$$F = V + L$$

$$F \cdot x_{CH4}^F = V \cdot x_{CH4}^V + L \cdot x_{CH4}^L$$

$$F \cdot x_{HC}^F = L \cdot x_{HC}^L$$

$$F \cdot x_S^F = L \cdot x_S^L$$

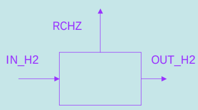
$$1 = x_{H2}^L + x_{CH4}^L + x_S^L + x_{HC}^L$$

$$1 = x_{H2}^V + x_{CH4}^V$$

$$x_{H2}^V = pv_{H2} \cdot (P^{\circ}_{H2}(T_F)/P_F) \cdot x_{H2}^L$$

$$x_{CH4}^V = pv_{CH4} \cdot (P^{\circ}_{CH4}(T_F)/P_F) \cdot x_{CH4}^L$$

Membranes – static model



ON

$$F_{IN\_H2} = F_{OUT\_H2} + F_{RCHZ}$$

$$F_{IN\_H2} \cdot x_{H2}^{IN\_H2} = F_{OUT\_H2} \cdot x_{H2}^{OUT\_H2} + F_{RCHZ} \cdot x_{H2}^{RCHZ}$$

$$x_{H2}^{OUT\_H2} = f(x_{H2}^{IN\_H2}, F_{RCHZ})$$

OFF

$$\frac{F_{RCHZ\_H2}}{F_{IN\_H2}} = 1$$

$$x_{H2}^{RCHZ\_H2} = x_{H2}^{IN\_H2}$$

METHODOLOGY FOR OFF-LINE PARAMETER ESTIMATION

1. - DATA RECONCILIATION

In order to take advantage of all the available measures

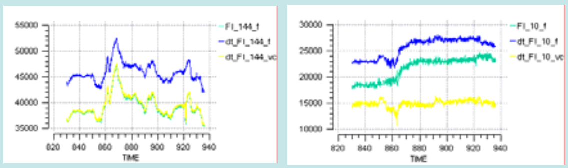
$$\min \sum_j (flow_j - flow_j^{vc})^2$$

- Extended to all the measured flowrates
- Model variable that fits balance perfectly
- Experimental value corrected by means of molecular weight obtained from model

- Redundant flowrate measures
- Flowrate measures of hydrogen streams corrected by means of operation temperature, pressure and molecular weight
- Molecular weights obtained from model and experimental correlations

Boundaries (inputs): $flow_j = flow_j^{vc} + bias$

Decision variable for the optimization problem to solve reconciliation



2. - CALCULATION OF PARAMETERS – Inverse model

- Experimental data of available measures corresponding to model output variables are used to identify the kinetic parameters of the model
  - H2 purity of the recycle stream from the high pressure flash drum
  - Outlet flow to fuel gas from low pressure separations
  - Sulfur concentration of the desulphurized hydrocarbon stream

3. - NEURAL NETWORK ARCHITECTURE

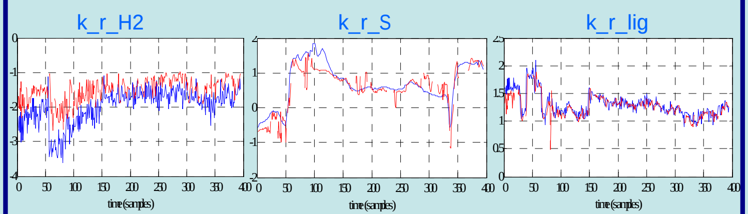
- Experimental data of external inputs are used as regressors for kinetic parameters estimation
  - H2 concentration in the reactor
  - Inlet temperature to the reactor
  - Flowrate fractions of different hydrocarbon mixed in feed

Trained with the Levenberg-Marquardt method.

NARX model
1st order in model outputs
2nd order in external inputs

3 NN
5 hidden hyperbolic nodes
1 output linear node

4. - NEURAL NETWORK VALIDATION



5. - FUTURE WORK – Implementation of NN in simulation

$$\min J = \sum_{t=1}^{N} \left(1/\sigma_i^2\right)\left[\hat{y}_i - y_i\right]^2$$

NOE model