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Self-optimizing control for hydrogen optimization in a diesel hydrodesulfurization plant

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Abstract

The aim of this work is to apply the self-optimizing control technique (Skogestad, 2000) in order to ascertain the plantwide control structure for a hydrodesulfurization HDS plant of a petroleum refinery with regards to hydrogen consumption optimization. The resulting control structure for the HDS plant is simple, robust to uncertainty, easy to implement (feedback control) and assures the global optimum in most cases, although an upper RTO layer will be needed to guarantee the operation in the adequate region, with non frequent updates. Only in one uncommon scenario a trade-off arises regarding the unconstrained degrees of freedom, and self-optimizing control variables must be looked for. Potential application to global refinery H_2 network is also discussed.

Keywords: self-optimizing control, hydrogen optimization, hydrodesulfurization plant.

1. Introduction

Hydrogen is an expensive utility used in many operations that is gaining increasing importance in the economic balance of a refinery. In this framework, a project oriented towards the optimal management of the real-time operation of a refinery H_2 network is being undertaken in collaboration with the Petronor refinery (Vizcaya, Spain) of the Repsol group (Sarabia et al., 2009), in order to minimize H_2 production costs.

H_2 is distributed by means of a network from the producer plants to the consumer plants. Make-up H_2 to each consumer plant can be provided from different production lines, corresponding to different producer plants as well as consumer plants outlets. Accumulation of H_2 is not possible; as a deficit of H_2 is very damaging for catalyst active life, being catalysts very expensive, then always H_2 production must exceed consumption in operation. Because H_2 is expensive to produce, minimization of H_2 production has a great potential for economic profit. Furthermore, in scenarios where H_2 production is bottleneck for the refinery fuel processing capacity, the potential for profit increase is even higher. Minimization of H_2 production cost is mainly achieved by means of: a) a better H_2 redistribution at the network scale, trying to reuse as much as possible the low purity H_2 from the consumer plants outlets; b) minimization of losses to fuel gas, as a consequence of a better fitting of H_2 production to H_2 consumption in operation, while guaranteeing certain excess for pressure control purposes.

Determining a good plantwide control structure, in this case for an H_2 consumer diesel hydrodesulfurization HDS plant, is an issue of great practical importance to achieve optimal operation. Skogestad's procedure looks for a control strategy which can be

implemented in practice in a robust and simple manner. In the first place, active constraints are controlled, and then, for the remaining unconstrained economic degrees of freedom, self-optimizing variables are looked for. Self-optimizing control (Skogestad, 2000) is when close-to-optimal economic operation is obtained with a constant set-point policy. In this way it is avoided, or at least reduced, the need for an upper optimization RTO layer, being feedback control still the easiest way to implement a control strategy in industrial practice (Skogestad, 2004). Self-optimizing control design has been applied successfully to many processes (e.g. Araujo, Govatsmark and Skogestad, 2007; Lid and Skogestad, 2008).

2. Hydrodesulfurization plant description

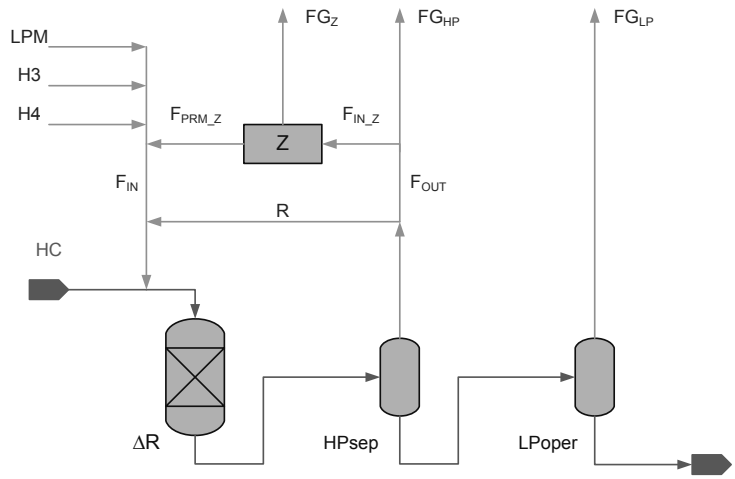

Figure 1. General H_2 consumer plant structure, with membranes unit for H_2 recovery.

A process flow diagram for the HDS plant is shown in Fig.1. Desulfurization reactions take place in fixed bed catalytic reactors (ΔR) where a minimum ratio H_2/hydrocarbon must be ensured for catalyst maintenance reasons. Reactors are fed with a blend of fuels of different qualities. The hydrocarbon (HC) feed is mixed with the recycled H_2 stream (R) and with make-up H_2 from the network. Two make-up streams (*H4*, *H3*) correspond to high purity inlets from producer plants, while the other (*LPM*) corresponds to the low purity line constituted from other plants outlets and excess. After being separated in a high pressure separation drum (*HPsep*), non reacted H_2 is partially recycled (R), partially purified and recycled in membranes Z (F_{PRM_Z}), and partially purged and burnt as fuel gas (FG_Z, FG_{HP}). Downstream of *HPsep*, several distillation columns at low pressure (*LPoper*) enable the complete separation of light gases from the desulfurized diesel stream. Light gases from low pressure separation processes (*LPoper*) are directed to fuel gas (FG_{LP}), since H_2 purity is not high enough for its recovery to be profitable. A HDS plant simplified model is available from previous work (Sayalero et al., 2010).

3. Self-optimizing control structure

The systematic procedure for plantwide control (Skogestad, 2004) will be applied to determine the self-optimizing control structure, following the steps in the top-down economic steady-state analysis.

3.1. Degrees of freedom analysis

A total of 5 degrees of freedom are available for economic optimization based on the process model. The following are natural manipulated variables (u) in operation: H_2 make-up flow rates from production plants F_{H3}, F_{H4}, membranes inlet flow rate F_{IN_Z}, membranes purge ratioed to the inlet F_{FG_Z}/F_{IN_Z}, purge to fuel gas from the high pressure recycle F_{FG_HP}. Other process variables are not truly degrees of freedom regarding H_2 optimization; that is the case for: a) pressure in separators, controlled at a fixed value according to compression ratios and security valves design; b) temperature in separators, regulated at minimum possible value by means of air exchangers, thus enabling the best relative separation of H_2 from light ends; c) quench flows between beds in the catalytic reactors, whose purpose is to maintain proper temperature gradients and to avoid high temperatures; d) reactor inlet temperature, which will always be active constraint at the minimum value enabling to achieve the sulfur specification in product.

3.2. Definition of optimal operation: cost and constraints

Only H_2 material cost is considered, as energy cost is in general an order of magnitude lower. Due to H_2 recycle flow being much greater than H_2 make-up flow, the H_2/hydrocarbon minimum ratio constraint (F_{H2}/F_{HC} > min) at reactor inlet is attained by means of recycle compressor's capacity (at minimum feasible, to minimize energy cost), and is thus decoupled from the H_2 optimization problem. Membranes operating costs can be disregarded as only low pressure steam is needed. Fuel gas value of purge streams is not considered (p_{fuel}) as this term will compete with minimization of the LPM make-up H_2 flowrate, being LPM H_2 price already a fictitious one. As a consequence, only make-up H_2 cost will be considered:

$$\min_u J = p_{H4} \cdot F_{H4} + p_{H3} \cdot F_{H3} + p_{LPM} \cdot F_{LPM} \qquad \text{(Eqn. 1.)}$$

Constraints to fulfill are the following: a) recycle H_2 purity between minimum to prevent deposition of coke over catalyst particles ensuring enough H_2 excess, and maximum to avoid surge of centrifugal compressor: min < y_{REC} < max; b) membranes operating range: min < F_{FG_Z}/F_{IN_Z} < max, and membranes capacity: min < F_{IN_Z} < max; c) producer plants capacity and LPM availability: min < F_{H3} < max, min < F_{H4} < max, 0 < F_{LPM} < max; d) compressors [reciprocating/centrifugal] capacity: min < F_C < max.

3.3. Identification of important disturbances

Regarding the plant state, disturbances in hydrocarbon feed influence: gas separated in the low pressure operations F_{FG_LP}, $y_{FG\_LP}^{H2}$, determined under pressure control according to inventory regulation; hydrogen consumption ΔR_{H2} and light ends generation ΔR_L in the reactor. Regarding different future scenarios, there are several disturbances that deserve being considered, namely: H_2 purity of certain make-up streams y_{LPM}^{H2}, y_{H3}^{H2}, and make-up availability from the low purity line F_{LPM}.

3.4. Regions of active constraints (modes of operation)

To identify the different regions of active constraints, optimization with respect to the available degrees of freedom is performed for the different operating points (19) selected corresponding to historical process conditions, for 6 case studies corresponding to different disturbances in utilities; in total 114 case studies. The model is implemented in EcosimPro® modelling and simulation environment and optimizations are performed with a NAG® SQP solver linked with EcosimPro®. In increasing order of H_2 requirements, the regions of active constraints are the following:

- **A.** Recycle H_2 purity (y_{REC}^{H2} = min) controlled with F_{IN_Z}. Manipulated variables active: F_{FG_Z}/F_{IN_Z} = min, F_{FG_HP} = 0, F_{H3} = 0, F_{H4} = 0.

The purge of H_2 is minimum (F_{FG_Z}/F_{IN_Z} = lower bound), and as a result both make-up H_2 flow and H_2 losses in the purge are also minimum.

- **B.** Recycle H_2 purity (y_{REC}^{H2} = min) controlled with F_{FG_Z}/F_{IN_Z}. Manipulated variables active: F_{IN_Z} = max, $F_{FG\_HP} = 0$, $F_{H3} = 0$, $F_{H4} = 0$.
  When H_2 requirements increase with respect to previous **A**, H_2 purge (F_{FG_Z}/F_{IN_Z}) is not at the lower bound because the membranes capacity upper bound is reached. Higher purge implies higher permeate purity, but also higher make-up H_2 flow rate.
- **C.** Recycle H_2 purity (y_{REC}^{H2} = min) controlled with F_{FG_HP}. Manipulated variables active: F_{IN_Z} = max, F_{FG_Z}/F_{IN_Z} = max, $F_{H3} = 0$, $F_{H4} = 0$.
  When H_2 requirements increase with respect to **B**, and membranes are saturated.
- **D.** Trade-off between ratio purged in membranes and HPM H_2 make-up (F_{H4}, F_{FG_Z}/F_{IN_Z}). Recycle H_2 purity controlled (y_{REC}^{H2} = min). Manipulated variables active: F_{IN_Z} = max, $F_{FG\_HP} = 0$, $F_{H3} = 0$. Case rather infrequent.
  When make-up H_2 from a producer plant (HPM H_2) is needed due to LPM H_2 shortage (small purity of 0.67 %1mol for example but not small F_{LPM} availability). The optimum is quite flat with respect to F_{FG_Z}/F_{IN_Z}, so a value can be fixed while using F_{H4} to control y_{REC}^{H2}, being $F_{FG\_Z}/F_{IN\_Z} = 0.33$ the most common by far (self-optimizing variable). According to the experiments carried out, the optimal ratio varies between 0.27-0.36, so 600 Nm^3 H_2/h is the difference for F_{IN_Z} = max, and the maximum loss in HPM H_2 is 300 Nm^3/h provided 0.33 is fixed. Cases B and D can be easily distinguished; if an increase in F_{LPM} (by allowing an increase in F_{FG_Z}/F_{IN_Z}) does not lead to an increase in y_{REC}^{H2}, then HPM H_2 will be needed. This occurs when $y_{LPM}^{H2} < y_{REC}^{H2}$. Direct purge F_{FG_HP} will be needed if membranes get saturated, besides HPM H_2.
- **E.** When the maximum make-up compressor's capacity is binding constraint besides y_{REC}^{H2} (y_{REC}^{H2} = min, F_{C1} = max), controlled with F_{FG_HP} and F_{H4}. Manipulated variables active: F_{IN_Z} = max, F_{FG_Z}/F_{IN_Z} = max, $F_{H3} = 0$.
  This situation is common in cases where $y_{LPM}^{H2} > y_{REC}^{H2}$, but only slightly greater. As a high flow F_{LPM} is needed, make-up compressor capacity gets saturated. As usual, membranes capacity is fully employed before HPM H_2 is used.
  F. When the maximum LPM H_2 availability is active constraint, besides y_{REC}^{H2} (y_{REC}^{H2} = min, F_{LPM} = max). Manipulated variables active: either F_{FG_Z}/F_{IN_Z} = min, $F_{FG\_HP} = 0$, $F_{H4} = 0$ (control with F_{IN_Z}, F_{H3}); F_{FG_Z}/F_{IN_Z} = min, $F_{FG\_HP} = 0$, $F_{H3} = 0$ (control with F_{IN_Z}, F_{H4}); F_{IN_Z} = max, F_{FG_Z}/F_{IN_Z} = min, $F_{FG\_HP} = 0$ (control with F_{H3}, F_{H4}); or F_{IN_Z} = max, $F_{FG\_HP} = 0$, $F_{H3} = 0$ (control with F_{FG_Z}/F_{IN_Z}, F_{H4}).
  Both membranes and HPM H_2 make-up are needed. With increasing H_2 demand, first F_{IN_Z} is manipulated, then F_{FG_Z}/F_{IN_Z}. Between the two HPM H_2, F_{H3} and F_{H4}, which one is used depends mainly on their respective prices and purities (very constant), but also on plant state, although no trade-off arises. An upper RTO layer will be required to know whether to use F_{H3} or F_{H4}, with very low frequent updates.

4. Discussion

Self-optimizing control is a robust technique not sensitive to uncertainty when compared with RTO (Skogestad, 2000). As i) disturbances: H_2 consumption, light gases inlet and generation, and gases solubility in hydrocarbons, are difficult to estimate accurately, and ii) gas flow measurements need to be compensated with molecular weight in operation, where the stream molecular weight is quite sensitive to light gases composition due to the low value of H_2 molecular weight (2.016 g/mol), a self-optimizing control approach can be advantageous and preferred compared to RTO.

Other major advantage is that the self-optimizing approach considered is reliable regardless of model mismatch: although model validation is not perfect quantitatively (errors up to 10% in the prediction of H_2 consumption rate), the analysis performed regarding regions of active constraints is correct.
The resulting control structure for the HDS plant is simple, easy to implement (feedback control with programmed logic) and assures the global optimum in most cases, although an upper RTO layer will be needed to guarantee the operation in the adequate region, with non frequent updates. Only in one scenario, rather uncommon, a trade-off arises regarding the unconstrained degrees of freedom, and self-optimizing control variables must be looked for to assure close to optimal operation avoiding more complex on-line optimization techniques. Main drawbacks are related to plant automation level, which needs to be high to implement this technology; in particular the membranes unit can't be operated manually. Transport delay due to reactor and dynamic effects due to separators are not negligible, therefore a MPC approach with an economic objective function could be justified, especially when the high number of regions of active constraints is taken into account, due to its potential to easily handle constraints.

4.1. Hydrogen optimal management at refinery network scale

A further step is being considered regarding the potential application of self-optimizing control design to on-line optimization of the global H_2 network operation. Although the structure at network scale is much more complex, the number of combinations allowed is usually small. Considering where it is more efficient to employ HPM H_2, and looking for self-optimizing variables when needed, consumer plants optimization with regards to H_2 consumption could be decoupled from the whole network, being the problem at network scale simplified, and thus reducing the loss between RTO executions.

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