Self-Optimizing Control Structure Design for a Staged Fischer-Tropsch GTL Process – Steady State Analysis

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Abstract

Optimization of a staged natural gas to hydrocarbon liquids (GTL) process while natural gas feed is also a degree of freedom is considered. The target is to design a self-optimizing control structure which works near optimum in a wide range of operation without the need to update the controlled variables (CVs) setpoints or change the control loops. Maximum possible throughput and the bottleneck of the process are found. The self-optimizing CVs are proposed for the optimal operation of this process.

Keywords: Staging, Maximum Throughput, Throughput Manipulator (TPM), Process Bottleneck

Introduction

Natural gas to hydrocarbons liquids process (GTL) is production of transportable liquid hydrocarbons from natural gas as feed. In this process, natural gas is first converted to a mixture of CO and H_2 which is called synthesis gas (syngas). In the next step, heavier liquids are produced from syngas in Fischer-Tropsch (FT) section. For final separation, hydrocarbon liquids are sent to upgrading and purification section [1]. Sulfur-free fuel is one of the best benefits of this process. Rafiee and Panahi studied staging a cobalt based FT reactor in a GTL

process in order to increase wax production rate [2]. Optimal operation of chemical plants is of great importance to achieve maximum profit while operational and environmental constraints are satisfied. Skogestad has developed self-optimizing procedure to systematically find the best controlled variables for optimal operation of chemical plants in present of unavoidable disturbances [3]. In the current paper, self-optimizing idea is applied on a staged FT GTL process to find the best controlled variables.

Process description

Syngas unit: natural gas feed and superheated steam enter pre-reformer at 3000 kPa and 455 °C. The aim of this section is converting of hydrocarbons heavier than methane to syngas to avoid cracking in subsequent ATR. Reaction schemes in pre-reformer are presented in Table 1 and named reforming (1), methanation (2) and water-gas-shift (3) respectively. A fired heater heats up the feeds to the pre-reformer and also outlet of the pre-reformer to 675 ^{0}C before entering the ATR. The oxygen is supplied by Air Separation Unit (ASU). ATR temperature reaches 1030 ^{0}C where high conversion of methane to syngas takes place. Syngas is cooled down through a steam boiler and a cooler in order to remove water content. A CO_2 absorber is also used to remove CO_2 from syngas before transferring it to Fischer-Tropsch (FT) synthesis section. The reaction schemes of the ATR are shown as equations 4,5 and 6 respectively.

Fischer-Tropsch (FT) section: In the slurry bubble column FT reactor (SBCR), which is approximated with a CSTR in our simulations, syngas is converted to a wide range of hydrocarbons through highly exothermic Fischer-Tropsch reactions. Reaction scheme is written as equation (7). Product distribution (eq. 8) and reactions rate are obtained from the Anderson-Schulz-Flory (ASF) model (eq. 9) and Iglesia et al [4] rates respectively. In the ASF model, α is chain growth probability, which is a function of hydrogen and carbon monoxide mole fractions in the SBCR and is calculated from eq. 10 [5, 6]. The details of how the GTL model has been simulated is given in the work of Panahi et. al. [7].

Table 1. Reaction schemes

$for\,(n\geq 2), C_nH_m + nH_2O \rightarrow (\mathrm{n}+\frac{m}{2})\mathrm{H}_2 + n\,\mathrm{CO}$	(1)	$CO + 3H_2 \rightleftharpoons CH_4 + H_2O$	(2)
$CO + H_2O \rightleftharpoons CO_2 + H_2$	(3)	$CH_4 + \frac{3}{2}O_2 \rightleftharpoons CO + 2H_2O$	(4)
$CH_4 + H_2O \rightleftharpoons CO + 3H_2$	(5)	$CO + H_2O \rightleftharpoons CO_2 + H_2$	(6)
$nCO + 2nH_2 \rightarrow (-CH_2-)_n + nH_2O$	(7)	$W_n = n(1-\alpha)^2\alpha^{n-1}$	(8)
$r_{CO} = \frac{k_2 {P_{H_2}}^{0.6} {P_{CO}}^{0.65}}{1 + K_1 P_{CO}}$	(9)	$\alpha = (0.2332\frac{y_{CO}}{y_{CO}+y_{H_2}} + 0.633)[1 - 0.0039(\mathrm{T}-533)]$	(10)

This study is continuation of the two previous works where control structure was designed for a single stage GTL process [8] and staging of the process was proposed [2]. The base case for the current work is taken from [2] where a two-stage FT reactor with the aim of maximizing wax flowrate was optimized. In this work, natural gas feed is also a degree of freedom and optimization is done with the objective of maximizing wax to find the bottleneck and

maximum possible throughput of the process. A self-optimizing control structure is proposed by finding the set of self-optimized controlled variables (SOC CVs).

Simulation, Results and discussion

Increase in natural gas feed from the economical point of view can lead in rise in GTL plant's profit [8]. However there are capacity limits (operation constraints) such as: duty of fired-heater (+40% compared to nominal case), feed rate to CO_2 removal unit (+20%), oxygen feed rate (+20%) and FT reactor volume [8] which should be noted while throughput increases.

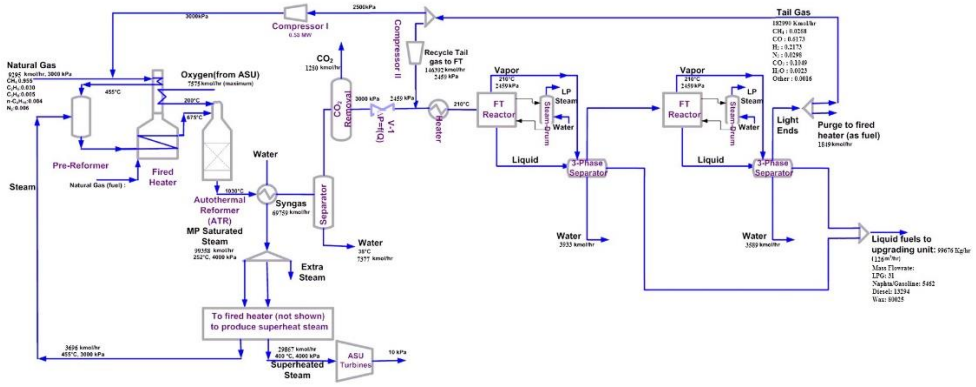

Figure 1: 2-Stage FT reactor in GTL flow sheet with data for optimal maximum throughput (point A in Fig. 2). Base flowsheet is taken from the work of Panahi and Skogestad [8]

Figure 2 reveals increase in re-optimized profit as a function of feed flow rate from nominal point up to point A when first capacity constraint (saturation of oxygen supply) is reached. Further increase in throughput is not recommended to avoid operation in snowballing region [8].

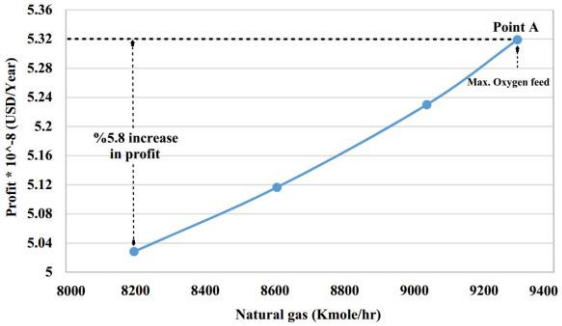

Figure. 2, Optimal profit as a function of natural gas flow rate. Point A

Self-optimized control structure

By re-optimization of the process, natural gas feed rate increases up to 13.4% where the profit increases to 5.8%. At this point oxygen flow rate becomes active. Active constraints are shown in Table1. The recycle ratio to FT ratio is remained optimally constant at 0.8 all over the re-optimization of the process and therefore it can be used as self-optimizing CV. Therefore we have 5 controlled variables with steady state effect, which need to be controlled.

Table1 : Active constraints (CVs), their optimum values and proposed MVs for pairing

CVs	optimum value	MVs
Fired heater outlet temperature of process stream to ATR	675 ^{0}C	Fired heater duty
ATR outlet Temp	1030 ^{0}C	Natural gas feedrate
Tail gas purge ratio	0.01	Split ratio
H_2O/C_{feed} to pre-reformer	0.4	Adjusting the steam flowrate to keep the ratio

At the maximum through put case (point A), there are 6 degrees of freedom (DOFs) with steady state effect on the objective function, which are: 1- steam to carbon ratio to the pre-reformer, 2- natural gas feedrate, 3- fired heater duty, 4- CO_2 recovery percentage, 5- tail gas purge ratio, 6- recycled tail gas split ratio to syngas unit and FT reactor. 4 of them are proposed to control the 4 active constraints as described in Table 1. Recycled tails ratio to syngas and FT unit is also kept constant at optimal value of 0.8 using split ratio. Therefore there is only one unconstrained DOF left, which is CO_2 recovery percentage. The setpoint for CO_2 recovery can be used as the throughput manipulator (TPM), which sets the production flowrate. This is shown in Fig. 3. CO_2 recovery percentage adjusts the H_2/CO ratio in syngas, which is indirectly sets the liquid product flowrate through chain growth probability in the FT reactor. Dynamic simulation is recommended to validate the proposed structure.

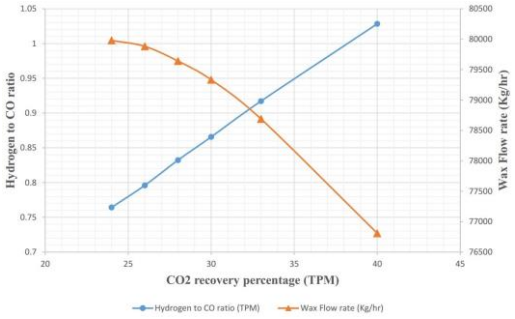

Fig. 3, change in wax flowrate an H2/CO in fresh syngas vs. change in CO2 recovery percentage

Conclusion

Self-optimizing is applied on a staged GTL process at maximum throughput case. There are 6 steady state degrees of freedom, which 5 of them are used to control 4 active constraints and 1 self-optimizing CV. There is one unconstrained DOF left, which is CO_2 recovery percentage. The setpoint of the unconstrained DOF is used as throughput manipulator.

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