INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 34 (2009) 9233–9238

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Reduced superstructure solution of MINLP problem in refinery hydrogen management

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ARTICLE INFO

Article history:
Received 29 January 2009
Received in revised form
28 August 2009
Accepted 28 August 2009
Available online 7 October 2009

Keywords:
Optimization
Hydrogen management
Refinery
Superstructure
Reduced superstructure
Mixed integer nonlinear programming
Genetic algorithm

ABSTRACT

Minimizing Hydrogen waste into fuel gas within the H_2 network in a refinery is the objective function of an optimization problem in this paper. The superstructure obtained for a refinery wide concept, is first solved and validated for literature cases, then is reduced by heuristic rules, based on engineering judgment. The reduced superstructure contains all simulation procedures of pseudo-components definitions, fine tunings of all unit operations to reach actual operating conditions, reactions characterization, linear and nonlinear equalities and inequalities as system constraints. The set of governing equations are solved with Genetic Algorithm. Based on this optimization, in an Iranian refinery 22.6% reduction of H_2 production and a saving of 1.19 million \$/year could be achieved.

1. Introduction

The world's energy demand, driven by the economic growth, is increasing at a high rate. The fossil fuels, as the most cost effective sources of energy production, are depleting. The viable alternatives should comply with the awareness of growing environmental concerns; among the criteria which make an alternative process-wise acceptable, one may name but a few: renewable, sustainable, efficient, cost effective and safe. Among politicians, environmentalists, and scientists an ongoing discussion is underway to accept and adopt the most suitable alternative process. The hydrogen has been expected as the most prominent resource [1]. Since the crude oil crisis waves of 70s and 90s, processes like electrolysis and coal gasification has emerged. But these processes are still under doubtful inspections for environmental or economical acceptance. Nevertheless any such decision should satisfy both "external" and "internal" interactions for "policy planning" and "managerial decision making" [2], while global warming and carbon-free nature of the process should be kept as a constraint.

As hydrogen can be found in nature only as compounds, a great amount of energy is needed to produce it [3]. Many authentic sources argue that hydrogen has the potential of overcoming its development obstacles including the global warming issue. They believe that hydrogen would be the fuel of future and it seems to solve the environmental issues as it looks to be a green energy carrier [4]. The hydrogen as a continuous and renewable energy source is one of the alternatives to succeed the current fossil fuels energy system.

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doi:10.1016/j.ijhydene.2009.08.086

Nomenclature

Symbols

C_P	heat capacity at constant pressure, J/kg °C
C_{Heat}	cost per unit of heat energy
F	flowrate, Kmol/h
H_2	Hydrogen
P	Pressure, Pa
T	Temperature, K
y	mole fraction of H_2
L	Lower bounds flow-rate which can be sent to new equipments
U	Upper flow-rate which can be sent to new equipments

Greek letters

ΔH^0	enthalpy of formation
ρ	density, kg/m^3
η	compressor efficiency
α	ratio of specific heats

On a long term basis, the substitution of fossil fuel by hydrogen will need a solid base large scale production process. The actual economically feasible process for large scale H_2 production is natural gas–steam reforming, mostly called steam–methane reforming (SMR) [5]. However in short-term time, the optimization and the improvement of existing hydrogen production technology is a necessity [6]. On the other hand, more strict environmental regulations and standards led refiners to increase the use of H_2. Thus, H_2 production, consumption and management in the industry, for a more efficient use of this valuable material, should be reconsidered thoroughly. Although the modification of each single process has merits, but the interaction between all integrated processes in a refinery, determines finally the system's performance.

One available option to ameliorate the H_2 distribution system is to increase its purity in one or more H_2 sources. The stream with higher H_2 purity will provide the system with more H_2 per unit flowrate. This surplus of H_2 will reduce the need of fresh H_2 production and increase the recycling [7].

Two main methods are practiced for an efficient H_2 management system: graphical (mainly to search for the pinch point) and mathematical approach.

Alves analyses the refinery H_2 distribution by graphical targeting approach [7]. Hallalea describes the superstructure method applying to the system for finding the optimal solution for H_2 distribution [8].

The main disadvantage of graphical approach is that it considers solely the purity and flowrates of streams, while the pressure of sources and sinks also has to be considered. In the case that the source's outlet pressure is less than sink's inlet, a compressor should be used to satisfy the destination pressure. Compressor is one of the major investment expenses in a refinery. However, this method will give a theoretical solution which is not necessarily applicable in a real system. On the other hand, this approach will find the minimum use of H_2, while the commercial and environmental aspects have to be considered as well.

2. Hydrogen management in a typical refinery

There are several processes for H_2 production in the refining industry and many applications where it is consumed. Among most common production processes are steam methane reforming (SMR) and partial oxidation (POX). In SMR process, the most widely used H_2 production route, a mixture of steam and methane flows in a fixed bed catalytic reactor to produce a mixture of H_2, CO_2 and CO, a mixture known as synthesis gas. The water gas shift reaction (WGS) produces an additional amount of hydrogen in two phases of high and low temperature [4]. The H_2 is separated from the mixture by different physical, like Pressure Swing Adsorption (PSA), or chemical processes like CO_2 and CO's chemical absorption by solvents.

3. Hydroprocessing

The Hydroprocessing is the major H_2 consumer. Lighter hydrocarbon cuts are richer in hydrogen, which in turn affects the Gasoline, Kerosene, and Diesel cuts quality. Tough regulations are the cause of most hydrogen-demanding sink within the overall H_2 balance in a refinery with an acceptable environmental impact [9].

Three products criteria have to be considered by refiners: lighter, higher performance, and environmentally acceptable. Sulfur and Nitrogen, as well as undesirable hydrocarbon components like aromatics, are removed by hydroprocessing to meet product specifications and satisfy environmental regulations [9].

4. Imperfections of superstructure

The main difficulty within the superstructure method is its complexity in real large networks which may cause the problem not to be solved at all. Therefore the system becomes so complicated and large that the existing problem solving tools are either inadequate or they require long time to get results. Conventional methods have difficulties like large computation, long CPU time, and also encountering local optima which makes them incompatible. In this paper it is suggested to reduce the superstructure with a sense of process engineering before applying the optimization methods. Thus, it is vital to remove some improper complexities without losing the accuracy, in addition to use some simplifying assumptions.

5. Formulation of objective function

Considering all possible connections between sources and sinks is necessary before formulating the objective function.