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# Modeling and optimization of an industrial hydrocracker plant

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ABSTRACT

The main objective of this study is modeling and optimization of an industrial Hydrocracker Unit (HU) using Artificial Neural Network (ANN) model. In this case some data from an industrial hydrocracker plant were collected. Two-thirds of the data points were used to train ANN model. Among the various networks and architectures, two multilayer feed forward networks with Back Propagation (BP) training algorithm were found as the best model for the plant. Inputs of both ANNs include fresh feed and recycle hydrogen flow rate, temperature of reactors, mole percentage of $H_2$ and $H_2S$, feed flow rate and temperature of debutanizer, pressure of debutanizer receiver, top and bottom temperature of fractionator column and pressure of fractionator column. The first network was employed to calculate the specific gravity of gas oil, kerosene, Light Naphtha (LN), Heavy Naphtha (HN), gas oil and kerosene flash point and gas oil pour point. The second network was used to calculate the volume percent of $C_4$, LN, HN and kerosene, gas oil and fractionators column residual (off test). Unseen data points were used to check generalization capability of the best network. There were good overlap between network estimations and unseen data.
In the next step of study sensitivity analysis was carried out on plant to check the effect of input variables on the plant performance. In this case temperature was found as the most affecting parameter in the plant. Finally optimization was performed to maximize the volume percent of gas oil, kerosene, HN and LN production and to identify the sets of optimum operating parameters to maximize these product yields. Optimum conditions were found as feed flow rate of 113.2 $m^3/h$, reactor temperature of 413 °C, hydrogen flow rate of 111.3 MSCM/h and LN () feed vol.% of 9.22.


## 1. Introduction

Hydro-cracking is a catalytic cracking process which has high conversion. Cracking conversion of a hydrocracker unit (HU) is more important than fluid cat cracking units and hydrogen partial pressure of the unit is higher than hydro-desulphurization processes (Maples, 2000).

In this process, hydrogen purifies the hydrocarbon stream from sulfur and nitrogen hetero-atoms. The process produces saturated hydrocarbons. The main products for HU are jet fuel and diesel, while also relatively high octane rating gasoline and LPG are produced. All these products have a very low sulfur content and other contaminants (Lyons, 2005).

The First Principle Models (FPMs) are common for the modeling the HU, but the complete development of these models can be very complex. Many industrial chemical and petrochemical processes are complex in nature typically due to unknown reaction chemistry, nonlinear relations and numerous involved variables (Bhutani et al., 2006b). Heavy and time-consuming computations are sometimes drawbacks of FPMs. Sometimes, in FPMs, complex partial differential equations or complex algebraic equations appear which should be solved analytically or numerically. Also, some phenomena, for example, kinetics of HU reactions are still not well-understood to develop an accurate mathematical model (Aguiar and Filho, 2001).

ANN modeling is a good alternative to FPMs to manage the complexities mentioned since it only requires the input-output data as opposed to a detailed knowledge of a system. In addition, ANN requires less computational time and allows estimation of every continuous and nonlinear function with high precision. because of these features ANN is very popular for modeling, simulation, optimization and control of processes in petrochemicals and refineries (Al-Enzi and Elkamel, 2000; Bellos et al., 2005; Bollas et al., 2003; Bollas et al., 2004; Falla et al., 2006; Shirvani et al., 2010; Zahedi et al., 2006; Zahedi et al., 2010).

Al-Enez and Elkamel have focused on predicting the effect of feedstock on the properties and the product yield for a Fluid Catalytic Cracking (FCC) unit. They used feed forward ANN to predict the yield of propane, butane, n-butane, iso-butane, propylene, butylene, light gas, gasoline, light cycle oil, heavy cycle oil, coke and carbon conradson number. Only four properties of feed including °*API*,

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## Nomenclature

| | |
|---|---|
| $a_k$ | kth node activation |
| *BP* | Backpropagation |
| *CGF* | Fletcher-Powell Conjugate Gradient |
| $f(x)$ | The output of the node |
| $f_i$ | Objective function for optimization |
| *F* | Feed flow rate (make up and recycle) |
| *H* | Inlet flow rate of hydrogen |
| *HN* | Heavy Naphtha |
| *HU* | Hydrocracker Unit |
| *LN* | Light Naphtha |
| *Mea.* | Measured data |
| *MLP* | Multi Layer Perceptron |
| *N* | Number of data |
| *Off test* | Residual Fractionator column |
| *p* | The parameter vector (for sensitivity analysis) |
| *RBF* | Radial Basis Function |
| *SCG* | Scaled Conjugate Gradient |
| *Sim.* | Simulated data |
| $t_k^p$ | *k*th node target pattern |
| *T* | Temperature of reactors |
| $w_{jk}$ | Weights |
| *x* | Sum of weighted inputs to the neuron |
| *y* | The state vector (for sensitivity analysis) |
| $x_{ki}^p$ | *k*th node input pattern |
| $y_k^p$ | *k*th node output pattern |

*Greek symbols*

| | |
|---|---|
| $a$ | Network learning rate |
| $\delta_k$ | Hidden layer kth node error |
| $\delta_j$ | Output *j*th node error |
| $\sigma$ | Transfer function |
| $\Delta w_{ki}$ | The error gradient |

Watson characterization factor, sulfur and volume conversion percent of liquid were introduced to NN as inputs. Their model gave better prediction than models from non-linear regression and commercial simulators (Al-Enzi and Elkamel, 2000).

An ANN hybrid model was used by Bollas et al., 2003 to scale up a FCC pilot plant into an industrial scale plant. The pilot model was able to predict the weight percent conversion and the coke yield. The hybrid model was then compared with the pilot model and the pure ANN model. The results showed that the hybrid model has better extrapolation capacity (Bollas et al., 2003).

Bellos et al., 2005 used a hybrid ANN model for hydrodesulphurization reactor modeling. They coupled the deterministic model which was used to study the reactor performance and hydrogen consumption, with an ANN model which was able to evaluate the kinetic parameters. The obtained results showed that the hybrid model was capable of predicting the reactor performance (Bellos et al., 2005).

The crude oil description using the near infrared spectroscopy was performed by Falla et al., 2006. This analysis was called SimDis (Simulation Distillation) and was faster than the true boiling point method. Forty oil samples with API of 1.31-36.4 were gathered. The ANN was applied, which generated the SimDis curves accurately (Falla et al., 2006).

An ANN model was used by us for simulation of an industrial Hydrotreater Unit. (Zahedi et al., 2006). we used Radial Basis Function (RBF) modeling as an optimum architecture to predict hydrogen demand, outlet API, and sulfur weight percent as a function of inlet API and sulfur weight percent for seven different feed stocks. A comparison between our model with the obtained results of a conventional simulator confirmed the superiority of the ANN model.

In another study we focused on enhancing the gasoline production of an industrial catalytic reformer unit. The ANN model anticipated the unit outputs accurately and led to 2,38% increase in gasoline production yield (Zahedi et al., 2008).

Aminian and Shahhosseini (2008) used ANN to predict the fouling behavior of a crude oil preheat heat exchangers. They also used sensitivity analysis known as the "sequential zeroing of weights" to determine the effects of various parameters on fouling (Aminian and Shahhosseini, 2008).

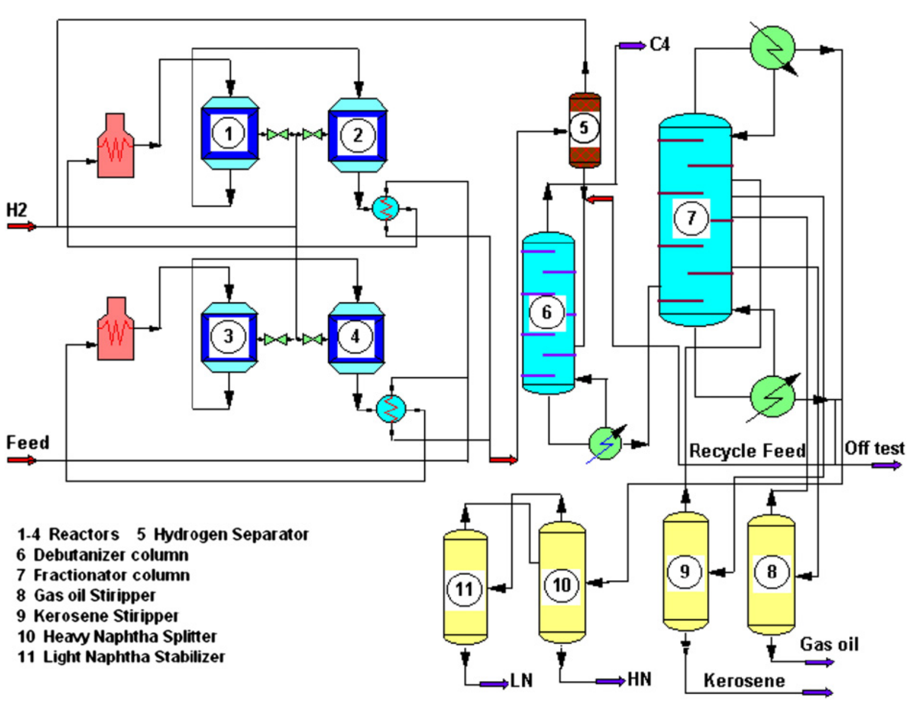


**Fig. 1.** Process flow diagram of a hydrocracking unit (Isomax unit).