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APPLICATION OF RESPONSE SURFACE METHODOLOGY IN THE SIMULATION AND ANALYSIS OF THE CATALYTIC CRACKING PROCESS IN A FLUIDIZED BED

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ABSTRACT: The fluidized catalytic cracking (FCC) process, also known as catalytic cracking, is one of the most valuable operations in the refining system due to the diversity and quality of the products obtained, which serve as feedstocks for various areas of the process complex. Operational deviations and supply deficiencies can compromise product quality. In this context, an alternative optimization strategy is proposed based on operational transition routes for different components of the *riser* outlet stream, including naphthenes, aromatics, olefins, paraffins, sulfur, and naphtha, as well as additional relevant parameters: coke formation, coke deposited on the catalyst, and overall conversion. The study considered vacuum gas oil feeds of 27,500, 30,000, and 30,250 BBD, processed at temperatures of 205, 368, and 532 °C and at pressures of 2.0, 2.5, and 3.5 $kg{\cdot}cm^{-2}$, in a *riser* 36.5 m high and 1.0 m in diameter. The Akzo A/F-3 catalyst was used, whose main composition by weight corresponds to 26.69% zeolite, 37.20% alumina, and 3.746×10^{-2}% rare earths, with standard selectivity characteristics. With these operating combinations, 27 simulation scenarios were established. Based on the results obtained, and using Microsoft Excel, linear and quadratic statistical models were adjusted to estimate values in intermediate sub-scenarios to the nine main scenarios for each response variable.

KEYWORDS: multivariable optimization, catalytic cracking, fluidized bed, response surface methodology

Introduction

Technological advances in the energy sector, driven mainly by the need to reduce environmental impact, have consolidated oil refining and the petrochemical industry as key players in the global economic landscape. Despite the growth of renewable energies, numerous petroleum derivatives remain indispensable in many regions, maintaining the strategic relevance of these processes. Technological evolution has changed the stability of the traditional market, as new energy demands drive the search for operational alternatives that improve efficiency and sustainability.

In this context, the fluid catalytic cracking (FCC) process is one of the fundamental stages in oil refining, as it allows heavy crude fractions to be transformed into light hydrocarbons with high commercial value (Khaldi et al., 2025). Both reactor and regenerator technology and catalyst design and formulation have evolved significantly, along with energy optimization strategies and emission mitigation systems. Similarly, operating conditions, critical process variables, and potential problems inherent in FCC operation have been the subject of ongoing study.

Description of the FCC process

The FCC process is characterized by its high capacity to convert vacuum gas oils and other heavy fractions into higher value products such as high-octane gasoline, liquefied petroleum gas (LPG), and light olefins (Figure 1). The conversion is based on endothermic catalytic reactions that occur at high temperatures and short residence times, where hydrocarbon chains are fragmented, isomerized, and cyclized to produce a diverse distribution of products (Alvarez & Saucedo, 2021).

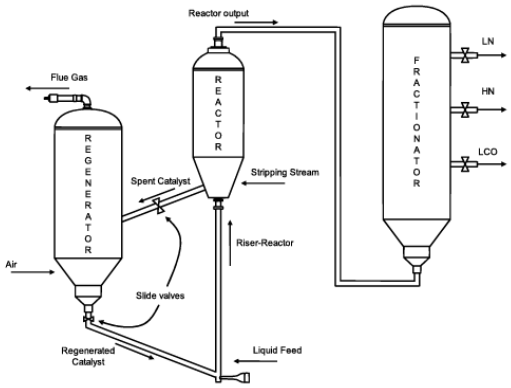

Figure 1. Representation of the FCC process (Khaldi et al. 2025)

The system operates through continuous contact between the vaporized feed and a finely divided solid catalyst, composed mainly of acidic zeolites supported on an alumina-silica matrix. The upward flow of vapors fluidizes the catalyst, creating favorable conditions for heat and mass transfer (Gary, Handwerk & Kaiser, 2007). The feed, usually hydrotreated to minimize impurities such as sulfur and metals, enters the riser where it reaches temperatures between 480 and 550 °C, causing rapid reactions that generate gasoline, LPG, dry gas, and coke (Sadeghbeigi, 2012).

The deposited coke reduces the acidity and activity of the catalyst, so it is sent to the regenerator, where it is partially burned at 650–720 °C to restore its activity and provide the heat required by the process (Speight, 2014). The regenerated catalyst returns to the riser, ensuring the cyclical nature of the system. The vaporized products are then sent to a fractionation column where the different commercial streams, including gasoline, LCO, and slurry oil, are separated.

Modern units incorporate advanced emission control systems, particle recovery, and pollutant reduction technologies, as well as catalytic improvements aimed at reducing coke formation and increasing selectivity to light olefins (Sadeghbeigi, 2012; Speight, 2014).

Advances in FCC process simulation and optimization

The increasing complexity of feedstocks and the challenges associated with maximizing the economic efficiency of the process have driven the development of advanced simulation and optimization tools. Since the late 20th century, mathematical modeling of FCC has become an essential strategy for understanding the interaction between reaction kinetics, mass transfer, and heat transfer in the reactor-regenerator (Sadeghbeigi, 2012).

In Mexico, the work of Ramírez Jiménez (2002), García Dopido (2004), and Zitlalpopoca Soriano (2005) stands out. They developed simulation models of the *riser,* the regenerator, and the complete FCC system based on actual operating conditions at national refineries.

The first models were based on global material and energy balances, together with simplified kinetic schemes based on *lumps*. With advances in computational capacity, detailed kinetic models of multiple *lumps* emerged, which were later integrated into commercial process simulators that allowed for the analysis of variations in feed, catalytic formulation, and operating severity (Gary et al., 2007; Speight, 2014).

Complementarily, Computational Fluid Dynamics (CFD) enabled the local characterization of flow patterns, thermal gradients, solid segregation, and reaction profiles within the *riser* and regenerator, leading to multiscale models with greater predictive power (Alvarez & Saucedo, 2021).

Optimization methodologies have evolved from classical mathematical programming techniques to heuristic algorithms such as genetic algorithms and particle swarm optimization, capable of exploring highly nonlinear decision spaces. In recent years, the incorporation of artificial intelligence and digital twins has enabled the development of hybrid models for real-time prediction and advanced predictive control (MPC), improving operational stability and efficiency (Alvarez & Saucedo, 2021).

Together, these advances consolidate simulation and optimization as essential elements for ensuring more efficient, flexible, and environmentally responsible operations in FCC units.

Methodology

Simulation scenarios

In this work, the maximum, intermediate, and minimum operating conditions of the FCC unit were identified (Table 1). Based on these values, **27 simulation scenarios** were generated**.**

Variable	Units	Value		
		Maximum	Intermediate	Minimum
Power	(barrels/day)	30,250	30,000	27,500
Temperature	(°C)	532	368	205
Pressure	(kg/cm^2)	3.5	2.5	2

Table 1. Operating conditions for the simulation

The process simulation was performed in Aspen HYSYS®, using the calib_one_riser.fcc template and the process diagram shown in Figure 2.

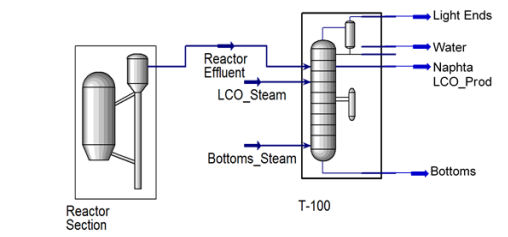

Figure 2. Simulation of the FCC process in Hysys

Statistical Modeling and Response Surface

Based on the simulation results, the methodology proposed by Velázquez et al. (2025) was applied to generate predictive models for each response variable: % coke and composition of olefins, paraffins, naphthenes, aromatics, and naphtha [%(v/V)].

The models used correspond to polynomial equations suitable for predicting responses as a function of independent variables (Veza et al., 2023). For k variables, the first-order linear model is expressed as shown in equation (1).

$$Y_i = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \varepsilon \qquad (1)$$

The second-order quadratic model has the form of equation (2).

$$Y_i = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i=1}^{k} \sum_{<j=1}^{k} \beta_{ij} x_i x_j + \varepsilon \qquad (2)$$

Where is the response variable "i", is the independent coefficient, also known as the average of responses, and and are coefficients of the statistical model, x_i are the independent variables, and$e$ is the statistical error.

Results

Simulation

The results of the 27 simulation scenarios are shown in Table 2.

Statistical models

Linear and quadratic models were obtained in order to determine which one best fit each variable analyzed, considering temperature and feed flow as independent variables. Table 3 shows the resulting equations and their correlation coefficients.

Analysis of results

The response surfaces generated from these models are shown in Figure 3.

Coke is essential for maintaining the thermal balance of the process. Figure 3a shows that the quadratic model predicts a maximum of **5.49%**, associated with **low temperature** conditions **(≈250 °C)** and **low feed flow (27,500 BPD)**.

With regard to olefins (Figure 3b), whose content increases octane rating and serves as a petrochemical feedstock, the highest concentrations are obtained between **450–500 °C** and **29,500–30,000 BPD**.

Figure 3c shows that high concentrations of paraffins are favored when both temperature and flow **decrease**, which is unfavorable due to its effect on reducing gasoline octane rating.

Figure 3d shows that naphthenes increase mainly with **temperature**, although there is also a slight dependence on flow. In the case of aromatics (Figure 3e), the best fit corresponded to the quadratic model; high concentrations are reached between **500–532 °C** and flows close to **30,000 BPD**.

Finally, naphtha (Figure 3f), one of the key products of FCC (Carrasco, 2010), has an estimated maximum close to **28,800 BPD** and **205 °C**, a behavior that is unique compared to the rest of the compounds analyzed.

Conclusions

When analyzing the values that the response variables take with each simulation, the following was observed:

- Four equivalent routes were established for each variable in order to facilitate the comparison and selection of optimal operating conditions.
- Pressure did not show a significant influence on product composition when temperature and flow were kept constant, as the results obtained were identical for each group of simulations.
- For all response variables except olefins, the quadratic model showed the best fit, so it was used to construct response surfaces and define operational transition routes.
- Gasoline is the relevant product, as it showed consistently higher values, making it the main variable under study.

Scenario	% Coke	Composition [%(v/V)]				Naphtha
		Olefins	Paraffins	Naphthenes	Aromatics	
1	5.49	49.84	34.67	9.321	6,176	57.3868
2	5.49	49.83	34.67	9.321	6,176	57.3868
3	5.49	49.84	34.67	9.321	6,176	57.3868
4	4.34	54.37	28.67	10.48	6.485	54.2347
5	4.34	54.37	28.67	10.48	6.485	54.2347
6	4.34	54.37	28.67	10.48	6.485	54.2347
7	2.61	62.61	13.79	13.35	7.249	45.2157
8	2.61	65.61	13.80	13.34	7.249	45.2157
9	2.61	65.61	13.79	13.35	7.249	45.2157
10	5.33	50.85	33.33	9.579	6.245	58.8393
11	5.33	50.85	33.33	9.579	6.245	58.8393
12	5.33	50.85	33.33	9.579	6,245	58.8393
13	4.21	55.57	27.07	10.78	6.567	53.4902
14	4.21	55.57	27.07	10.78	6.567	53.4902
15	4.21	55.57	27.07	10.78	6,567	53.4902
16	2.53	67.21	11.68	13.75	7.358	44.0796
17	2.53	67.21	11.68	13.75	7.358	44.0796
18	2.53	67.21	11.68	13.75	7.358	44.0796
19	5.32	50.95	33.20	9,604	6,252	56.7843
20	5.32	50.94	33.20	9,604	6,252	56.7843
21	5.32	50.92	33.20	9,604	6,252	56.7843
22	4.20	55.69	26.92	10.82	6.575	53.4157
23	4.20	55.69	26.92	10.82	6.575	53.4157
24	4.20	55.69	26.92	10.82	6.575	53.4157
25	2.52	67.37	11.47	13.79	7.368	43.9674
26	2.52	67.37	11.47	13.79	7.368	43.9674
27	2.52	67.37	11.47	13.79	7.368	43.9674

Table 2. Simulation results

Model	Equation	Correlation coefficient
%coke		
Linear	$Y = -0.00864598x_1 - 4.88288E^{-5}x_2 + 8.673957$	0.987
Quadratic	$Y = -0.003660258x_1 - 1.044E^{-5}x_1^2 - 0.00027859x_2 + 3.39394E^{-9}x_2^2 + 9.25929E^{-8}x_1x_2 - 0.51871$	0.999
Olefins [%(v/V)]		
Linear	$Y = 0.048508104x_1 + 0.000633514x_2 + 20.9851706$	0.994
Quadratic	$Y = -0.095853152x_1 + 0.000121x_1^2 + 0.00314391x_2 - 5.5596E^{-8}x_2^2 + 1.88588E^{-6}x_1x_2 + 9.489748$	0.941
Paraffins [%(v/V)]		
Linear	$Y = -0.065529225x_1 - 0.000672673x_2 + 68.34597709$	0.945
Quadratic	$Y = 0.086203193x_1 - 0.0001682x_1^2 - 0.000752051x_2 + 7.43434E^{-9}x_2^2 - 9.4806E^{-7}x_1x_2 + 44.44114$	0.999
Aromatics [%(v/V)]		
Linear	$Y = 0.003367391x_1 + 3.45946E^{-5}x_2 + 4.44500793$	0.945
Quadratic	$Y = -0.004405417x_1 + 8.6282E^{-6}x_1^2 + 4.47603E^{-5}x_2 - 4.84848E^{-10}x_2^2 + 4.82855E^{-8}x_1x_2 + 5.58163$	0.999
Naphthenes [%(v/V)]		
Linear	$Y = 0.01262789x_1 + 0.000128817x_2 + 2.85535383$	0.945
Quadratic	$Y = -0.016449208x_1 + 3.2376E^{-5}x_1^2 - 0.00018463x_2 + 4.29899E^{-9}x_2^2 + 1.7814E^{-7}x_1x_2 + 12.16042$	0.999
Naphtha [%(v/V)]		
Linear	$Y = -0.040534041x_1 - 0.000215559x_2 + 73.1699818$	0.939
Quadratic	$Y = 0.082496931x_1 - 9.90483E^{-5}x_1^2 + 0.061875138x_2 - 1.06613E^{-6}x_2^2 - 1.70995E^{-6}x_1x_2 - 840.890$	0.994

Table 3. Linear and quadratic models for response variables

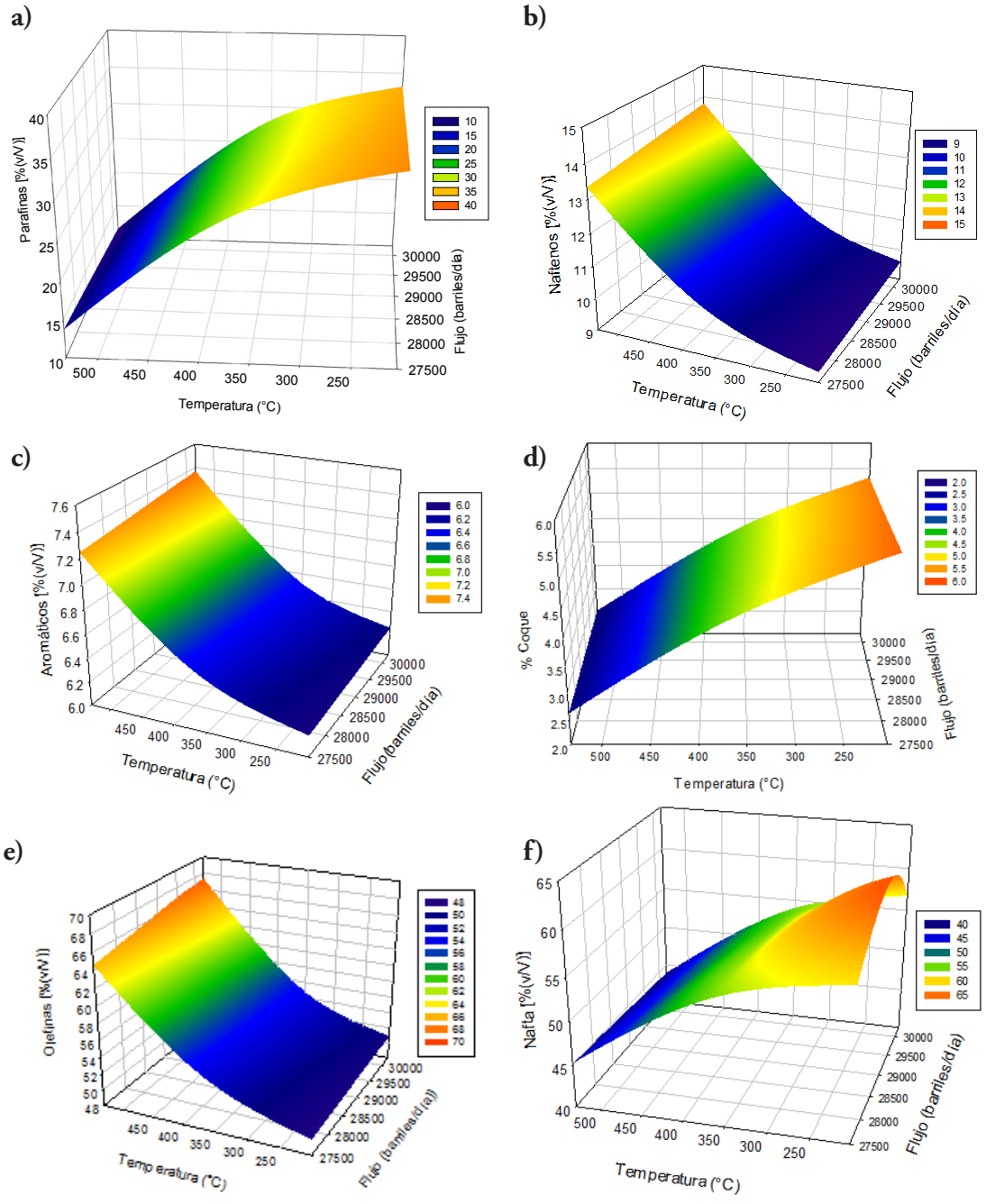

Figure 3. Response surface graphs for a) % coke, b) olefins [%(v/V)], c) paraffins [%(v/V)], d) naphthenes [%(v/V)], e) aromatics [%(v/V)] and f) naphtha [%(v/V)]

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