Ciencia Digital

ISSN: **2602-8085**
Vol. 8 No. 3, pp. 47 – 63, julio – septiembre 2024

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Molecular optimization in fluid catalytic cracking process: cartesian coordinate analysis for enhancing efficiency and quality in crude oil refining

Optimización molecular en el proceso de fluid catalytic cracking: análisis de coordenadas cartesianas para mejora de eficiencia y calidad en la refinación de crudo

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Artículo de Investigación Científica y Tecnológica
Enviado: 15/04/2024
Revisado: 10/05/2024
Aceptado: 10/06/2024
Publicado:05/07/2024
DOI: **https://doi.org/10.33262/cienciadigital.v8i3.3079**

Cítese: Trávez Osorio, S. E., Nacimba Rivera, N. O., Robalino Cacuango, M. J., & Moreno Corrales, A. S. (2024). Optimización molecular en el proceso de fluid catalytic cracking: análisis de coordenadas cartesianas para mejora de eficiencia y calidad en la refinación de crudo. Ciencia Digital, 8(3), 47-63. https://doi.org/10.33262/cienciadigital.v8i3.3079

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Ciencia Digital
ISSN: **2602-8085**
Vol. 8 No. 3, pp. 47 – 63, julio – septiembre 2024
www.cienciadigital.org

Palabras claves:
formación vocacional, orientación profesional, carreras técnicas, estudiantes de media superior.

Resumen

Introducción: En el refinado de petróleo crudo, el proceso de craqueo catalítico fluido (FCC) convierte el petróleo crudo en productos petroquímicos de alta calidad. Comprender las interacciones moleculares en FCC es crucial para fines de optimización, eficiencia y calidad. Este estudio cuantitativo y descriptivo analiza las coordenadas cartesianas de compuestos clave, empleando química computacional para este propósito. **Metodología**: Cuantitativa y descriptiva. A través de una revisión de la literatura, se identificaron compuestos químicos típicos que alimentan el proceso de FCC, incluidas parafinas, olefinas, aromáticos y naftenos, entre otros. Estos compuestos se procesaron mediante química computacional para obtener sus coordenadas 3D, optimizando su geometría molecular para representar la estructura real, garantizando una precisión confiable de los datos en simulaciones y análisis posteriores. **Análisis y discusión de resultados**: Las coordenadas cartesianas ayudan a comprender e identificar las condiciones operativas óptimas, mejorando la comprensión de las interacciones moleculares en tiempo real y facilitando la predicción de comportamientos de separación. Estas coordenadas están previstas para optimizar los procesos de refino de crudo en FCC, mediante la modelización y visualización de movimientos y colisiones a nivel atómico. **Conclusiones**: La optimización de la geometría molecular utilizando el campo de fuerza apropiado es crucial para obtener coordenadas cartesianas precisas. Estas coordenadas permiten la simulación de interacciones moleculares a nivel atómico, el diseño de catalizadores más eficientes y la optimización de procesos de refinado. Además, el monitoreo en tiempo real con datos moleculares precisos podría garantizar una calidad constante del producto en FCC.

Keywords:
Cartesian coordinates, Fluid Catalytic Cracking (FCC), refinery, computational chemistry,

Abstract

Introduction: In crude oil refining, the Fluid Catalytic Cracking (FCC) process converts crude oil into high-quality petrochemical products. Understanding molecular interactions in FCC is crucial for optimization, efficiency, and quality purposes. This quantitative and descriptive study analyzes Cartesian coordinates of key compounds, employing computational chemistry for this purpose. Methodology: Quantitative and descriptive. Through a literature

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optimization energy.

review, typical chemical compounds feeding into the FCC process were identified, including paraffins, olefins, aromatics, and naphthenes among others. These compounds were processed using computational chemistry to obtain their 3D coordinates, optimizing their molecular geometry to represent the real structure, ensuring reliable data accuracy in subsequent simulations and analysis. Analysis and Discussion of Results: Cartesian coordinates aid in understanding and identifying optimal operating conditions, enhancing the comprehension of molecular interactions in real time and facilitating the prediction of separation behaviors. These coordinates are envisaged to optimize crude oil refining processes in FCC, through modeling and visualization of atomic-level movements and collisions. Conclusions: Optimizing molecular geometry using the appropriate force field is crucial for obtaining precise Cartesian coordinates. These coordinates enable the simulation of molecular interactions at the atomic level, design of more efficient catalysts, and optimization of refining processes. Additionally, real-time monitoring with accurate molecular data could ensure consistent product quality in FCC.

Introduction:

Crude oil refining is a complex process that involves transforming crude oil into high-quality petrochemical products. At the core of this refining process lies Fluid Catalytic Cracking (FCC), which enables the production of high-demand fuels and chemicals. However, understanding the molecular interactions within this process is crucial for optimizing efficiency and product quality.

In this context, there is a growing need to increase the yield of refinery products, such as LPG, gasoline, and other high-octane products, in both national and international markets. Consequently, there is a demand to contribute to scientific development through theoretical-computational studies of chemical species reported in various bibliographic sources.

How can the Cartesian coordinates of molecules influence the optimization of crude oil refining processes?

The objective of this article is to analyze the Cartesian coordinates of key compounds in the FCC process and explore their implications for process optimization and

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understanding molecular interactions. Understanding the Cartesian coordinates of molecules is crucial for comprehending how molecules interact in the FCC process, thereby enabling the optimization of efficiency and product quality. Additionally, molecular dynamics simulations allow us to predict how molecules interact with each other, facilitating the modeling and visualization of these atomic-level movements and collisions. This knowledge is vital for understanding how molecules transform during catalytic processes, allowing for precise simulations of the chemical reactions that occur during crude oil refining.

The justification for this study lies in the importance of understanding the Cartesian coordinates of molecules to comprehend how they interact in the FCC process, thereby enabling the optimization of efficiency and product quality. The methodology used in this study is quantitative and descriptive, relying on the compilation and analysis of data through a comprehensive literature review and subsequent analysis using computational chemistry techniques.

This approach aims to yield relevant results for identifying and analyzing the Cartesian coordinates of key compounds in the FCC process, thus generating information on how to optimize efficiency and the quality of the final product. The aim is to contribute to the existing knowledge in the field of crude oil refining by presenting a detailed analysis of the Cartesian coordinates of key compounds in the FCC process.

Methodology

Chemical Compound Identification

Through bibliographic research, typical chemical components found in the feed streams to the FCC process have been identified. According to the blend of light and heavy gas oil known as Vacuum Gas Oil (VGO), it is used as the feed stream to FCC catalytic plants to produce high-octane gasoline. Additionally, the feed includes paraffins, olefins, aromatics, and naphthenes, each of which is fed to its corresponding E-Cat D catalyst at the appropriate temperature. (Sadeghbeigi, 2020) .

The raw materials for feeding the FCC unit for vacuum gas oil and atmospheric residue consist of sulfur, nitrogen, nickel, and vanadium residues, each in different weight percentages. The feed stream to the FCC process, Vacuum Gas Oil B (VGB-B), with E-Cat D catalyst at a temperature of 500°C, includes paraffins ranging from methane (CH_4) to dodecane ($C_{12}H_{26}$), iso-butane, iso-pentane, iso-hexane, iso-heptane, iso-octane, iso-nonane, and iso-decane, as well as paraffins from carbon 20-27 in various weight percentages. Olefins range from ethylene (C_2H_4) to decene ($C_{10}H_{20}$). Aromatics such as benzene, toluene, and C_8H_8 aromatics are present, each in different weight percentages. For the feeds of FCC for Light Cycle Oil (LCO) and VGO, benzene, decalin,

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tetralin, naphthalene, 1-phenyloctane, biphenyl, fluorene, 9,10-dihydrophenanthrene, phenanthrene, pyrene, and benzo(a)anthracene are present, all ranging between 98 and 99% in weight (Chiluisa Cando, 2021) (Nazarova y otros, 2022).

Similarly, naphthenes with feed positions to the FCC unit include cyclopentane, cyclohexene, 1,1,2-trimethylcyclopentane, phenanthrene, cyclopentyl methyl ether, cyclohexane, and methylcyclohexane (Stratiev y otros, 2023). Additionally, the author (Chiluisa Cando, 2021) also reports bromobenzene, fluorobenzene, methylbenzene, nitrobenzene, hydroxybenzene, vinylbenzene, tert-butylbenzene, 1,2-dichlorobenzene, 1-Bromo-3-nitrobenzene, 1-ethyl-4-isopropylbenzene, 1-ethyl-2-methylbenzene, 1-ethyl-3-methylbenzene, 1,4-dimethylbenzene, 1-bromo-2,3-dimethylbenzene, and 1,2,4-trinitrobenzene.

Computational chemistry information processing

Through computational chemistry data processing, each molecule was processed to individually obtain the 3D coordinates of the chemical compounds. Initially, these coordinates are unoptimized. This was achieved using Avogadro, which is an advanced molecule editor and visualizer software designed for multi-platform use in computational chemistry (Avogadro, 2024).

Initially, the generation of chemical structures in 2D was carried out using (ChemDraw, 2024) , which in computational chemistry is known for its efficiency, precision, and aesthetic appeal in chemical drawing. This program was chosen because it reduces errors in drawing, analyzing, and documenting the complex chemical structures presented in this study. To generate a chemical structure in 2D, the following steps were followed: using "Convert Name to Structure" within the Structure menu of ChemDraw, the name of the chemical compound in English was entered. As a result, the molecule was generated in line-angle format along with its English name. Once saved from ChemDraw in .mol format, the document was then opened in the Avogadro software.

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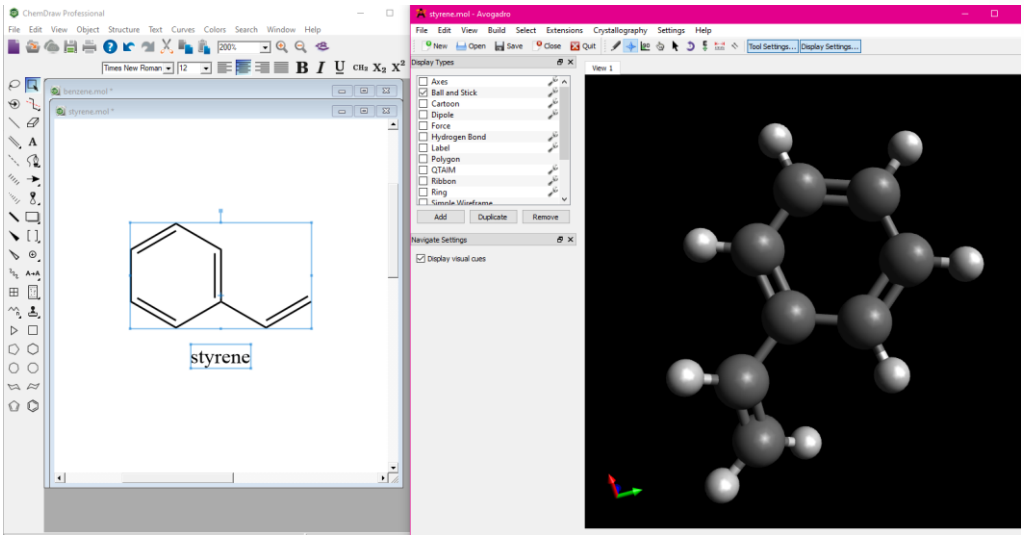
Figure 1

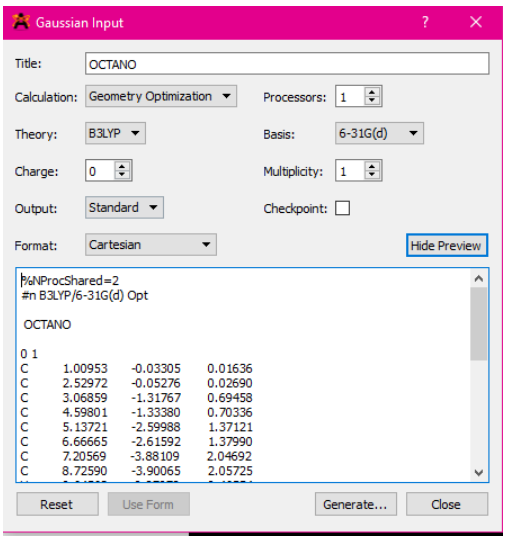
Processing of styrene molecule in computational chemistry.



(Avogadro, 2024) It is an open-source and free-to-use software that allows for the creation and visualization of molecular structures in 3D. Since this study was conducted using computational chemistry, this program proved to be a useful tool. Additionally, it enables the visualization of chemical structures from any angle. To obtain the Cartesian coordinates of each chemical compound, the Gaussian extension tool was selected from the Avogadro toolbar. This provided the unoptimized Cartesian coordinates (3D) of the analyzed chemical compound.

Figure 2

Non-optimised 3D octane coordinates



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Why should the molecule be optimised?

Gaussian calculations have various applications, including single-point energy calculations, optimization, and stability, among others (Chaurand Padilla y otros, 2022). Since this study will focus on molecule optimization, it delves into said optimization prior to obtaining their Cartesian coordinates. The importance lies in the fact that molecules are not always in the most stable geometry, so it is crucial to ensure that their spatial arrangement is accurate and represents the real molecular geometry (Paniagua & Mota, 2008) . On the other hand (San Fabián, 2023) mentions that molecule optimization involves adjusting the positions of atoms to minimize the total energy of the molecule, ensuring that the geometry is the most stable and representative of the analyzed chemical compound.

The equilibrium geometry is the configuration in which the molecule's energy is minimized, and this is considered the real geometry of the molecule. Without optimizing the molecule, the Cartesian coordinates may not reflect the real geometry, leading to errors in the calculations and subsequent analysis of the analyzed chemical compound (Chaurand Padilla y otros, 2022) (San Fabián, 2023) (Paniagua & Mota, 2008). Therefore, in the Avogadro toolbar, the AutoOptimization Setting was selected, and the force field was chosen to initiate this calculation, which may take seconds or a few minutes depending on the molecule being analyzed. For instance, in the case of cyclopentane, this analysis took several minutes to complete.

Why the choice of force field?

The choice of a force field for energy optimization in molecules is crucial in computational chemistry, considering that force fields are mathematical models that describe the forces and energy interactions between atoms and molecules in a system (Grabowski, 2020). Furthermore (Jorgensen & Tirado-Rives, 2005), selecting the appropriate force field ensures accuracy and realism in representing molecular interactions, optimizes molecular geometry, enables realistic dynamic simulations, facilitates the calculation of energetic and thermodynamic properties, and effectively handles the complexity of large systems (Vangunsteren & Berendsen, 1990).

What is the force field for hydrocarbon analysis??

he choice of the appropriate force field depends on the chemical nature of the molecule being optimized. For hydrocarbon analysis, the Merck Molecular Force Field (MMFF94) is commonly used (Avogadro, 2024), as this model optimizes the geometry of organic compound molecules. The MMFF94 has been specifically parameterized for alkanes, alkenes, alcohols, phenols, ethers, aldehydes, ketones, etc. Although the Universal Force Field (UFF) reproduces the most important structural characteristics across the periodic

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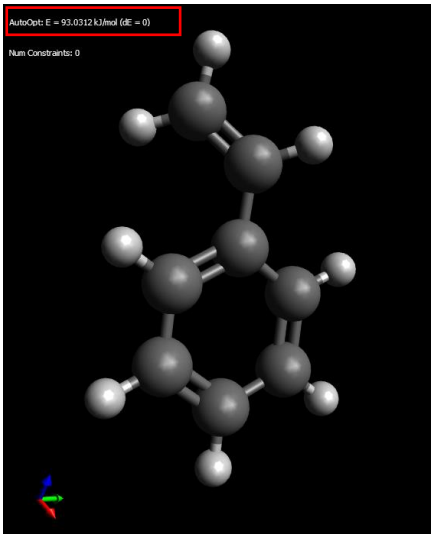
Vol. 8 No. 3, pp. 47 – 63, julio – septiembre 2024

table and optimizes geometry for all elements, including inorganic and organometallic materials. In this study, the MMFF94 was utilized for the analysis of the mentioned hydrocarbons.

Furthermore, the General AMBER Force Field (GAFF) model is employed for optimizing the geometries of drugs, while Assisted Model Building with Energy Refinement (AMBER) is used for protein analysis. (Avogadro, 2024).

Figure 3

Optimized Styrene Spatial Arrangement



RESULTS

For the paraffins fed into the FCC process, the coordinates of isobutane and octane are presented, respectively.

Table 1

Optimized molecule of isobutane and octane

Optimised isobutane molecule			
Atom	**Axis X**	**Axis Y**	**Axis Z**
C	0.88820	0.00508	0.02995
C	2.41498	-0.00393	0.00094
C	2.93829	-1.40974	-0.28513
C	2.93813	0.98548	-1.03797

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Table 1

Optimized molecule of isobutane and octane (continuation)

Optimised isobutane molecule			
Atom	**Axis X**	**Axis Y**	**Axis Z**
H	0.51003	-0.68214	0.79416
H	0.46936	-0.29844	-0.93561
H	0.50991	1.00590	0.26358
H	2.78062	0.30618	0.98749
H	2.60076	-1.76937	-1.26318
H	2.58859	-2.11661	0.47471
H	4.03328	-1.42567	-0.27793
H	2.60059	0.72086	-2.04589
H	4.03312	1.00281	-1.04123
H	2.58831	1.99991	-0.81917

Optimized Octane Molecule			
Atom	**Axis x**	**Axis y**	**Axis z**
C	0,84430	-0,00360	0,02940
C	2,36450	0,01060	0,01190
C	2,90350	0,91290	-1,09790
C	4,43290	0,92440	-1,11200
C	4,97240	1,82730	-2,22260
C	6,50180	1,83890	-2,23670
C	7,04080	2,74110	-3,34660
C	8,56100	2,75540	-3,36400
H	0,48060	-0,65480	0,83030
H	0,44460	-0,37600	-0,91920
H	0,44450	1,00100	0,20030
H	2,73210	-1,01260	-0,12840
H	2,73200	0,35690	0,98490

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Table 1

Optimized molecule of isobutane and octane (continuation)

Optimized Octane Molecule			
Atom	**Axis x**	**Axis y**	**Axis z**
H	2,52960	1,93410	-0,95520
H	2,52960	0,56470	-2,06850
H	4,80660	-0,09680	-1,25490
H	4,80660	1,27280	-0,14140
H	4,59860	2,84860	-2,07980
H	4,59870	1,47900	-3,19320
H	6,87580	0,81770	-2,37940
H	6,87570	2,18710	-1,26620
H	6,67320	3,76430	-3,20630
H	6,67330	2,39480	-4,31960
H	8,96070	3,12790	-2,41540
H	8,92480	3,40650	-4,16500
H	8,96080	1,75080	-3,53480

From the olefin stream feeding into the catalytic cracking process, propylene has been selected.

Table 2

Cartesian coordinates of propylene.

Molécula optimizada de propeno			
Atom	**Axis x**	**Axis y**	**Axis z**
C	0,98040	0,01740	0,10550
C	2,47390	0,01880	0,11420
C	3,20030	0,20230	1,22710
C	4,69390	0,20760	1,25910
H	0,61420	-0,15040	-0,91250
H	0,58670	0,97920	0,44800

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Table 2

Cartesian coordinates of propylene (continuaction)

Molécula optimizada de propeno			
Atom	**Axis x**	**Axis y**	**Axis z**
H	0,58670	-0,78360	0,73860
H	2,97070	-0,13860	-0,84040
H	2,69680	0,35920	2,17880
H	5,12990	0,04430	0,26850
H	5,05490	-0,58170	1,92550
H	5,05490	1,16910	1,63680

Representative of aromatic compounds is presented in the Cartesian coordinates of benzene and styrene.

Table 3

3D Cartesian coordinates of benzene and styrene

Optimised molecule							
Benzene				**Styrene**			
Atom	**Axis x**	**Axis y**	**Axis z**	**Atom**	**Axis x**	**Axis y**	**Axis z**
C	-0.76191	1.17879	-0.00445	C	1.07396	-0.39151	0.14829
C	-1.39352	-0.06483	-0.00378	C	2.17773	0.27468	-0.21451
C	-0.63232	-1.23364	-0.00582	C	2.89018	0.08040	-1.48472
C	0.76049	-1.15882	-0.00852	C	3.53569	1.17648	-2.07260
C	1.39211	0.08480	-0.00919	C	4.24873	1.02908	-3.26537
C	0.63091	1.25361	-0.00716	C	4.33389	-0.21939	-3.87721
H	-1.35497	2.08942	-0.00287	C	3.71074	-1.32081	-3.29475
H	-2.47868	-0.12313	-0.00168	C	2.99694	-1.17280	-2.10221
H	-1.12442	-2.20257	-0.00529	H	0.59741	-0.18466	1.10148
H	1.35356	-2.06946	-0.01011	H	0.60680	-1.13713	-0.48637

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Table 3

3D Cartesian coordinates of benzene and styrene (continuation)

Optimised molecule							
Benzene				Styrene			
Atom	**Axis x**	**Axis y**	**Axis z**	**Atom**	**Axis x**	**Axis y**	**Axis z**
H	2.47727	0.14309	-0.01130	H	2.58357	1.03246	0.45192
H	1.12301	2.22253	-0.00768	H	3.48122	2.15971	-1.61084
				H	4.73772	1.88947	-3.71450
				H	4.88933	-0.33505	-4.80411
				H	3.78350	-2.29819	-3.76442
				H	2.53569	-2.05050	-1.65687

Cyclopentane has been chosen for the naphthenes

Table 4

Optimised coordinates of the optimised cyclopentane molecule

Molécula optimizada de ciclopentano			
Atom	**Axis x**	**Axis y**	**Axis z**
C	-0.79462	-0.99232	-0.13821
C	0.72550	-1.05298	0.00185
C	1.20335	0.39253	0.12994
C	0.00632	1.24828	-0.25510
C	-1.17664	0.43179	0.23498
H	-1.29800	-1.73278	0.49065
H	-1.07619	-1.19392	-1.17871
H	1.17051	-1.54138	-0.87185
H	1.01893	-1.63169	0.88443
H	2.07563	0.59714	-0.49812
H	1.48803	0.59476	1.16947
H	-0.03909	1.36684	-1.34416
H	0.04387	2.24343	0.19695
H	-2.11907	0.74349	-0.22408
H	-1.27706	0.52371	1.32293

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The raw materials for the feed to the FCC unit for vacuum gas oil and atmospheric residue are presented in 3D coordinates of nitrogen and nickel and vanadium.

Table 5

3D coordinates of nitrogen, nickel and vanadium.

Optimised nitrogen molecule			
Atom	**Axis x**	**Axis y**	**Axis z**
N	0,86180	-0,03060	0,08760
N	2,28180	-0,03060	0,08760
Optimised nickel molecule			
Atom	**Axis x**	**Axis y**	**Axis z**
Ni	0.96824	-0.02527	-0.09139N
Optimised vanadium molecule			
Atom	**Axis x**	**Axis y**	**Axis z**
V	0.97576	0.08384	-0.04882

Analysis and discussion

Due to the FCC process with VGO-B and E-Cat D catalyst, the key compounds are paraffins (C_1-C_{12}), olefins (C_2-C_{10}), aromatics such as benzene, toluene, styrene, naphthenes such as cyclopentane, cyclohexene, as well as heavy compounds such as sulphides, nitrogen, nickel and vanadium. They have been considered as the most relevant due to their reactivity, coke formation, influence on catalyst selection and final product quality. (Nazarova y otros, 2022) (Stratiev y otros, 2023).

In crude oil refining processes, understanding the Cartesian coordinates of molecules can be important in several respects due to the complexity and accuracy needed to optimise processes and maximise efficiency. In molecular dynamics simulations, foresee how molecules interact with each other. Cartesian coordinates allow modelling and visualisation of these motions and collisions at the atomic level. On the other hand, coordinates provide knowledge to understand how molecules are transformed during catalytic processes, which would facilitate simulations of the chemical reactions that occur during crude oil refining (Zhang y otros, 2020).

The FCC unit operates by passing a zeolite catalyst along with feed vapor through a vertical reactor for a few seconds. The cracking products are separated from the solids

ISSN: **2602-8085**
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and directed to a distillation column to be divided into 25 desired products. The catalyst is recirculated to the regenerator, where accumulated coke is burned off, and the catalyst is regenerated for reuse (Fahim y otros, 2009). Therefore, understanding the positions of atoms in catalysts and reactants can help design more efficient catalysts. Similarly, analyzing how crude oil molecules interact with catalysts at the atomic level would be useful for improving reaction rates and selectivity (Zhang y otros, 2020).

Cartesian coordinates enable a precise representation of how molecules are distributed and move, along with their corresponding optimization energy for process optimization. This could identify optimal operating conditions (temperature, pressure, etc.) by better understanding molecular interactions and movements (Zhang y otros, 2020). Therefore, understanding molecular geometry helps predict and control separation behaviors, as it improves purification and separation techniques through detailed analysis of the involved molecules (Borges y otros, 2007) Furthermore, real-time monitoring could be enhanced using precise molecular data to adjust process parameters and maintain product quality (Yan & Duan, 2022).

Conclusiones

- The optimization of molecular geometry using the appropriate force field is a crucial step before obtaining Cartesian coordinates, as it ensures that these coordinates accurately represent the real molecular structure and minimize the molecule's energy. Moreover, a well-chosen force field enhances the reliability and validity of results obtained in computational studies.
- Utilizing Cartesian coordinates in molecular dynamics simulations allows for the prediction and visualization of how molecules interact at the atomic level in a realistic manner. Consequently, they can be employed to understand molecular transformations during catalytic processes in crude oil refining, such as FCC, thereby facilitating the simulation of chemical reactions and process optimization.
- Having a precise understanding of atomic positions in catalysts and reactants through molecular geometry aids in designing more efficient catalysts. In the case of FCC, the interaction between the feedstock and catalysts is crucial for process efficiency. Analyzing interactions between crude oil molecules and catalysts at the atomic level can enhance reaction rates and selectivity, resulting in a more effective fluid catalytic cracking process.
- Lastly, delving into computational chemistry allows for detailed knowledge of molecular geometry and motion, facilitated by Cartesian coordinates. This leads to identifying optimal operating conditions to improve purification and separation techniques, thus optimizing refining processes. Additionally, real-time monitoring using precise molecular data enables the adjustment of process parameters to maintain the quality of refined products.

ISSN: **2602-8085**
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Conflict of interests

There is no conflict of interest in relation to the article presented.

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Ciencia Digital

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Vol. 8 No. 3, pp. 47 – 63, julio – septiembre 2024

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