Physical Chemistry
ISSN: 0974-7524

Physical Chemistry: An Indian Journal

Research | Vol 12 Iss 1

Study of the Catalytic Activity of the Faujasite from Natural Clinker and Pumice

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Received: January 04, 2017; **Accepted:** February 02, 2017; **Published:** February 07, 2017

Abstract

The physical properties of faujasite obtained from natural black, red clinker and pumice were studied for subsequent replacement in base catalysts of zeolite type Y. To this end, sodium hydroxide was added as an alkaline activator to each of the raw materials. The resulting product was calcined and dissolved in distilled water, then transferred to a reactor where it was allowed to time for 24 hours and subjected to a hydrothermal treatment at 80°C for 12 hours. For the physical characterization, X-ray diffraction, Fourier transform infrared spectroscopy, particle size, TGA thermogravimetry and BET surface area using the Canonical Monte Carlo method were used to simulate the crystal structure of a theoretical faujasite, obtaining the BET that was compared with him of the experimental faujasite. The experimental results showed us that the zeolite obtained corresponds to faujasite and the crystallization of this one is directly proportional to the time of hydrothermal treatment. Finally, faujasite with a high content of amorphous material was obtained, despite its low proportion of crystal formation, its catalytic activity is reflected in its active centers that were quantified in a thermogravimetry balance.

Keywords: ***Zeolites; Faujasite; Heavy crude; Catalysts; Clinker***

Introduction

In petroleum industry, in refining area and in different chemical transformation processes, catalysts are used for their ability to increase the reaction rate and decrease the activation energy required for the transformation, at the same time, the catalyst has a high cost of acquisition that represents a great economic investment. This work focuses on the synthesis of faujasite from the natural clinker and pumice stone making use of alkaline fusion prior to hydrothermal treatment. Previously, there have been syntheses of zeolitic materials from natural clinker which is a residue from the coal exploitation generated from the natural combustion of the coal mantles as a consequence of the thermal alteration, resulting in the obtaining of different types of Zeolitic materials such as Sodalite and Faujasite. To reduce the high investment cost of the Esmeraldas State Refinery (REE) for the acquisition of the catalyst, especially the equilibrium, it is proposed the study of the use of faujasite in a natural state of easy acquisition at economic price [1,2].

The study of faujasite, type zeolite in its natural state, aims to study the possibility of substitution of the type Y zeolite currently used in the catalyst for the FCC unit. To identify the products synthesized from black and red natural clinker and pumice stone, analytical techniques were use, such as: X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-

Citation: Jimenez E*, Paucar A, and Herrera P. Study of the Catalytic Activity of the Faujasite from Natural Clinker and Pumice. Phys Chem Ind J. 2017;12(1):106.

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IR), particle size analyzer, area Superficial BET, and TGA thermogravimetry. In addition, using the Gran Canonical Monte Carlo (GCMC) method of the MEDEA software, the analytical technique of the BET surface area of the theoretical faujasite was carried out to compare with the natural faujasite [3,4]. X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FT-IR) showed that the zeolite obtained corresponds to faujasite in the three raw materials, identifying a higher percentage of faujasite in Clinker natural 2 (red) Concluding that the crystallization time of the zeolitic material was not sufficient to obtain a high percentage of zeolite. Experimentally, it was shown that faujasite possesses catalytic activity, obtaining a larger generation of cracked gases with a zeolite/crude ratio of 0.01.

1. Theory

Zeolites

Zeolites are highly crystalline hydrated aluminosilicates which upon dehydration develop, an ideal crystal, is a porous structure with minimum pore diameters of 3 to 10 angstroms. The zeolites can be natural or synthetic according to their origin:

Natural Zeolites

They are part of the group of minerals with a tetrahedral crystalline structure formed by Si and Al atoms. They are found in deposits of hydrothermal origin, cavities and fissures of volcanic rocks or in masses of sedimentary origin.

Synthetic Zeolites

They are created artificially for certain purposes. They are produced by hydrothermal synthesis and can include elements such as P, Ga, Ge. Ti, alkali metals, alkaline earth metals, lanthanides and even noble metals.

Zeolite Type Faujasita: "Faujasite is a natural mineral of great interest as a catalyst.

The basic unit of the faujasite is the regular cuba-octahedron or sodalite, which consists of 24 tetrahedra of SiO_{44}- or AlO_{45}. In FIG. 1, a representation of the structure of a Zeolite (a) type A (b) Type X or Y.

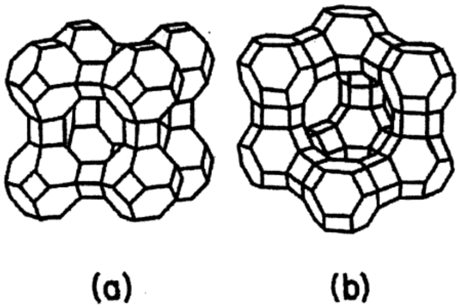


FIG. 1. **Structure of a zeolite Y.**

A feature of these structures is that they have very large cavities joined by small holes, have a very large surface area, with fixed geometry pores [4-6].

The size of the holes between cavities determines the size of the adsorbent molecule that can be accessed. The ability of a structure to adsorb some molecules and to reject others is the basis for the action of molecular sieves.

Fourier Transform Infrared Spectroscopy (FTIR) spectra corresponding to the zeolitic products obtained from the hydrothermal treatment of natural clinker in alkaline solutions

The typical bands of the zeolitic materials are: the asymmetric voltage of T-O (T = Al or Si) located in the region 950-1250 cm^{-1}, and the symmetric voltage of T-O located in the region 660- 770 cm^{-1}. Bands in the 500-650 cm^{-1} region are related to the presence of double rings (D4r and D6r) in the structure of the zeolitic materials. The bands in the region 420-500 cm^{-1} represent internal T-O vibrations, while the bands in the 300-420 cm^{-1} region are related to pore opening.

Secondary building units

According to Breck in 1974, the secondary units of construction are based on the type of secondary structural unit. They are divided into seven groups (FIG. 2):

(1) Single rings 4

(2) Single rings 6

(3) Rings 4dobles

(4) Double rings 6

(5) Complex units 4-1 [T_5O_{10}]

(6) Complex units 5-1 [T_8O_{16}]

(7) Complex units 4-4-1 [$T_{10}O_{20}$]

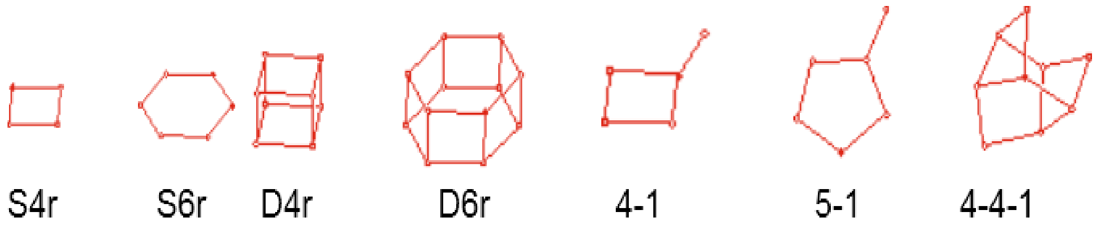


FIG 2. **Secondary building units.**

BET theory of the surface area test

It is called BET theory by the surnames of the creators, Brunauer, Emmett and Teller. It is based on the active forces in the condensation of the gases, they are also responsible for the bonding energy of multimolecular adsorption. By equalizing the rate of condensation of gas molecules on a layer already adsorbed at the rate of evaporation of that layer and summing for an infinite number of layers. We can see in the next expression [7,8].

$$N_a = \frac{n_m C P}{(P_0 - P)\left[1 + (C-1)\left(\frac{P}{P_0}\right)\right]} \qquad (1)$$

Na is obtained where P_0 is the constant saturation pressure of the gas. The value of C is:

$$C = \ exp^{\frac{q_1 - q_L}{RT}} \qquad (2)$$

Where q_1 represents heat of adsorption of the first layer, q_L means the heat of liquefaction of the adsorbent, R the typical gas constant, and T the absolute temperature in kelvin degrees.

Equation (1) can also be written in the linear form.

$$\frac{P}{N_a(P_0 - P)} = \frac{1}{n_m C}\ \frac{C-1}{n_m C}\left(\frac{P}{P_0}\right) \qquad (3)$$

In this case, a zone of $\frac{P}{N_a(P_0-P)}$ Vs $\frac{P}{P_0}$ we must produce a straight line with a slope.

The values of n_m and C can be obtained from an area of a straight line, or regression line, through the point.

Dynamic behavior of the catalysis process

Next, the dynamic behavior of the catalyst and zeolite process in different ratio is determined [9].

This behavior is represented by the variable R (t), indicating the ratio of catalyst/zeolite and has the following form:

$$\mathrm{R(t)} = \frac{1 - \mathrm{P(t)}}{\mathrm{P(t)}} \qquad (4)$$

In general:

The probability function in the Fisher Kolmogorov's equation given by P_ (k (T (x, y, x, t)) satisfies the Eikonal 3 equation of the optics, which represents the heat equation, if and only if a function exists F (x, y, z, t)> 0 and in addition $to\ \frac{\partial P\_<0}{\partial t}$.

$$\begin{Bmatrix} \frac{\partial P_{\_}}{\partial t} - \nabla^2 P_{\_} = kP_{\_}(1 - P_{\_})\,;\ 0.5 < P_{\_} < 0.823 \\ \frac{\partial T}{\partial t} - \nabla^2 T = 0;\ (x, y, z)\epsilon\, R;\ T, t\, \epsilon\, R^+ \\ |\nabla \mathrm{T}| = F(\mathrm{x}, \mathrm{y}, \mathrm{z}, \mathrm{t}) > 0;\ (x, y, z)\ \epsilon\, R;\ T, t\, \epsilon\, R^+ \end{Bmatrix} \tag{5}$$

Where P_ has the logistic probability density, such that.

$$P_{\_} = \frac{1}{1 + exp^{-kt}} \tag{6}$$

In the case of a first-order reaction, the concentration has the form:

$$C_{\_} = C_0 exp^{-\mathrm{k(T)t}} \tag{7}$$

Finally the concentration as a function of probability is:

$$C_{\_} = C_0 \frac{1 - P_{\_}}{P_{\_}} \tag{8}$$

Software Medea@2.15

This software predicts properties of solid materials using simulations based on quantum mechanics, statistical and mechanical thermodynamics. It contains licenses such as MEDEA-GIBBS, MEDEA-LAMMPS and MEDEA-PHONON.

The basic principle applies to systems in thermodynamic equilibrium, the method to simulate adsorption is the large canonical set or fluid phase equilibrium with the Gibbs set. The method used in this work is Monte Carlo which allows to construct statistical sets in thermodynamic equilibrium, but does not include dynamic properties of matter such as diffusion, viscosity or thermal conductivity [10,11].

The crystal structure was obtained from the program database which was simulated using the Monte Carlo Grand Canyon Method (GCMC) with the MEDEA-GIBBS license, to determine the BET surface area of the pore type (s) of the zeolite type Faujasite the program used N_2 nitrogen at 77 K, this was done with the aim of later comparing it with the experimental surface area.

Grand Canyon Monte Carlo (GCMC) or μVT

For pure compounds or multicomponent systems, temperatures and partial pressures are imposed to simulate a given point in the adsorption isotherm.

The most convenient statistical set is the large canonical set, also called the μVT set.

At low pressure, the chemical potential μi is linked to the partial pressures $P_i = Py_i$ where P is the total gas pressure and i is the mole fraction of component i.

The general expression implies fugacity f_i in the fluid phase in equilibrium with the adsorbent, which are equivalent to the partial pressure at the low pressure limit:

$$\mu_i = \mu_{i0} + RTIn\,\frac{f_i}{P_0} \approx \mu_{i0} + RTIn\,\frac{y_i P}{P_{0\ldots}} \qquad (9)$$

Where P_0 is a reference pressure. The chemical potential of each species appears explicitly in the probability of each state of the system in the great canonical set, which is proportional to:

$$\exp(\beta E_i + \beta N_1\mu_1 + \beta N_2\mu_2 + \ldots) \qquad (10)$$

A large canonization simulates the average number of molecules <Ni> in the system for each species i.

In the case of microporous adsorbents, this is the average number of adsorbed molecules.

The heat of adsorption can also be calculated [11-13].

Specific Movements of the Gibbs Assembly

The Gibbs Monte Carlo set (GEMC) involves two simulation frames with no explicit interface; specific movements are used in addition to single cell movements:

Coupled volume changes that provide mechanical balance (equal pressures in both phases).

Transfers

The transfer of molecules, whose objective is to impose equal chemical potential in both phases.

The probability of acceptance for the transfer of a molecule of type i from box A to box B is:

$$\mathrm{p}_{\mathrm{a}\infty}(\text{transfer } \mathrm{i}_{\mathrm{A}\to\mathrm{B}}) = \min\left[1, \frac{\mathrm{N_i^A}}{\mathrm{V^A}}\frac{\mathrm{V^B}}{\mathrm{N_i^B}}\exp\left(-\beta\left(\mathrm{U_{new}^A} - \mathrm{U_{old}^A} + \mathrm{U_{new}^B} - \mathrm{U_{old}^B}\right)\right)\right] \qquad (11)$$

Where the variables have the same meaning as in the above equations, the superscripts A and B refer to the phase in question.

Similar to insertions and suppression motions, GEMC transfers have a low probability of acceptance when one or both phases are particularly dense, or when large molecules are involved.

Volume changes

In the imposed pressure Gibbs set, the volume change movements are applied independently in each simulation box, and the acceptance probability is the same as equation (12).

$$p_{a\infty}(\mathrm{old} \rightarrow \mathrm{new}) = \min\left[1, \left(\frac{V + \Delta V}{V}\right)^{N} \exp(-\beta(U_{\mathrm{new}} - U_{\mathrm{old}}) - \beta P \Delta V)\right] \qquad (12)$$

This ensures that the simulation is performed at the requested pressure.

In the set of Gibbs at global volume imposed V = V A + V B, the volume changes ΔV are applied in phase A and -ΔV in phase B.

The probability of acceptance is:

$$p_{a\infty}(\Delta V) = \min\left[1, \left(\frac{V^{A} + \Delta V}{V^{A}}\right)^{N^{A}} \left(\frac{V^{B} - \Delta V}{V^{B}}\right)^{N^{B}} \exp\left(-\beta\left(U_{\mathrm{new}}^{A} - U_{\mathrm{old}}^{A} + U_{\mathrm{new}}^{B} - U_{\mathrm{old}}^{B}\right) - \beta P \Delta V\right)\right] \qquad (13)$$

Adsorption simulation algorithm in the Grand Canonical Monte Carlo set (GCMC)

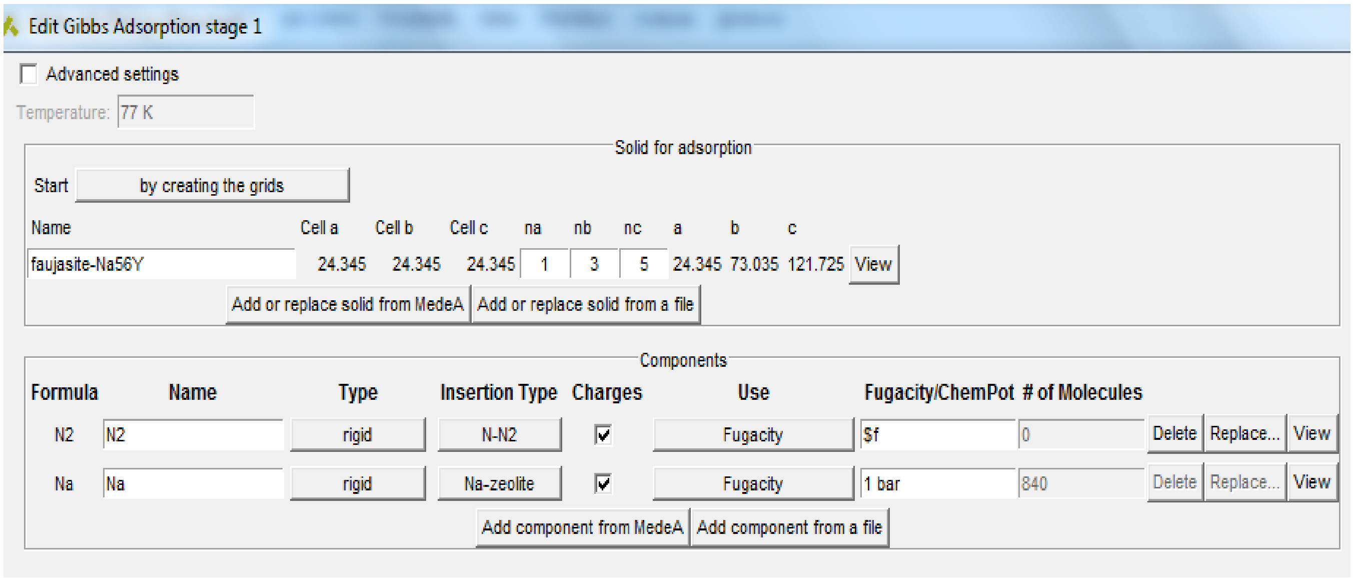
In the Great Canonical simulation, the flow diagram of the Gibbs adsorption editor specifies the chemical potential of each molecular species, as it is a parameter imposed on this set.

Alternatively, fugacity can be introduced, which is equivalent to the partial pressure at low pressure, rather than chemical potential.

The unit of chemical potential is Kelvin and the fugacity can be introduced as mPa, Pa, kPa, bar, atm in MEDEA® GIBBS.

The potential energy is recorded at the nodes of a grid with regular spacing at x, y, z of the cell unit of the crystal. The use of a larger simulation table of the unit cell is possible through panel parameters na, nb and nc (integer values). The resulting length of the simulation cell along, directions a, b, and c is provided. A small model is created and it assigns the strength field parameters and then uses a larger cell containing n × n × nc cells.

It is performed automatically after all necessary parameters have been defined and the solids input file has been provided in the Gibbs adsorption editor.



Edit Gibbs Adsorption stage 1

☐ Advanced settings

Temperature: 77 K

Solid for adsorption

Start: by creating the grids

Name	Cell a	Cell b	Cell c	na	nb	nc	a	b	c
faujasite-Na56Y	24.345	24.345	24.345	1	3	5	24.345	73.035	121.725

Components

Formula	Name	Type	Insertion Type	Charges	Use	Fugacity/ChemPot	# of Molecules
N2	N2	rigid	N-N2	☑	Fugacity	$f	0
Na	Na	rigid	Na-zeolite	☑	Fugacity	1 bar	840

FIG. 3. **Gibbs absorption editor.**

Medea lists the identified solids or molecules, and asks you to select the adsorbates in the component step (FIG. 3).

To simulate click on RUN.

2. Experimental Section

2.2. Equipment

2.2.1. **BET surface area analyzer:** This equipment was used to determine the surface area of the zeolitic material and is based on BET theory. Brand Horiba. Model SA-9600.

2.2.2. **X-Ray diffractometer:** This technique was used to obtain information on the structure and composition of the crystalline material. Brand Bruker. Model: D2 PHASER.

2.2.3. **Particle size analyzer:** was performed for the measurement of solid particle size, which is based on the per-camera recording of the projection of particles passing through a beam of light. Mark Retsch. Model Camsizer.

2.2.4. **Infrared Fourier Transform (FTIR) spectroscopy equipment:** for the characterization of the absorption bands of the raw materials and of the products obtained. Brand Perkin Elmer, Model Spectrum two.

2.2.5. **Termogravimétria (TGA):** this equipment determined the mass loss of heavycrude as a function of time [12]. Brand: METTLER TOLEDO. Model: GC200

2.2.6. **Mill:** used for crushing the natural clinker black and red, and pumice [13].

2.2.7. Muffle furnace: It was used to obtain the alkaline products using the different raw materials together with the sodium hydroxide. Thermo Scientific Brand. Polytetrafluoroethylene

2.2.8. Reactor: It is used for the formation of zeolite crystals Volume of 100 mL.

2.2.9. Magnetic stirrer: It is used to homogenize the reaction gel.

2.2.10. Stove: It is used for the hydrothermal treatment and drying of faujasita, range: (0-300) ° C Apą ± 1 ° C.

2.3. Materials

In order to carry out the process of alkaline fusion of zeolites, natural clinker 1 (black) and pumice stone were taken as raw materials from areas of the Chasquis-Cotopaxi mining complex and natural clinker 2 (red) from the Pintag sector, Quito.

The heavy crude of the Esmeraldas Refinery, 24 ° API, 23 ° of sulfur, Distilled water, Sodium hydroxide, 99.9% Sigma Aldrich

2.4 Method

The synthesis procedure was carried out by alkaline fusion followed by a hydrothermal treatment, for the crystallization of the zeolitic material. This process was repeated for the three raw materials [14-16].

A) Grind the starting material in a mill.

B) Initially mix 100 grams of sodium hydroxide (NaOH) in pellets with natural clinker, maintaining an alkaline activator/raw material ratio of 1.2/1, until a homogeneous mixture is obtained.

C) Calcine the resulting product at 600°C for 1 h, in a muffle oven and then allow to cool to room temperature.

D) Dissolve the fused alkaline product in distilled water (water/fused alkaline ratio = 5 mL/ g).

E) Shake the alkaline solution at 1100 rpm for 30 min until a homogeneous hydrogel is obtained; This reaction hydrogel was transferred to a 100 mL Teflon (PTFE) reactor.

F) Leave the hydrogel at rest for 24 hours, for off aluminization.

G) Subjecting the hydrogel to a temperature of 80°C for a time of 12 hours, thus obtaining a hydrothermal treatment.

H) Wash and filter the material obtained with distilled water until a pH of 7 is obtained in the filtrate in order to remove excess sodium hydroxide.

I) Dry the samples in an oven at 60°C for 1 hour.

J) In the thermogravimetry equipment create a method for each reaction temperature; program a dynamic thermal process as indicated in the following TABLE 1.

TABLE. 1**. Catalytic cracking thermal process.**

Terms	**Units**	**Value**
25°C a	°C/min	10
T° Reaction	minutes	30
Atmósphere	mL/min	75
Inert (N_2)		

K) Take a sample of the mixture and put it in the cell of the equipment for analysis.

L) Repeat this process for all the asphalt/catalyst ratios and the different reaction temperatures.

M) Determine the catalytic cracking zone and calculate the area under the curve for each of the tests.

3. Results and Discussion

Following are the results of the Faujasite 1 synthesized material obtained from the natural black Clinker as FAU-1, Faujasite 2 obtained from the natural red Clinker as FAU-2 and Faujasite 3 obtained from pumice as FAU-3.

3.1. Results of the Fourier transform infrared spectroscopy test

The FTIR spectra of the products obtained show that dehydration was not performed (H_2O deformation bands at 1634 cm^{-1}, 1643 cm^{-1} and 1634 cm^{-1}). However, for absorption at 923 cm^{-1}, 994 cm^{-1} and 991 cm^{-1} are associated with the asymmetric stretching vibration bands of the T-O bond (T = Si or Al), and the bands at 685 cm^{-1}, 676 cm^{-1} and 679 cm^{-1} belong to the Symmetrical vibrations of stretching T-O, finally the bands at 566 cm^{-1}, 558 cm^{-1} and 565 cm^{-1} belong to the resonances of the secondary structure D6r of the Faujasite (TABLE 2).

TABLE. 2. **Main bands of the FTIR spectra of the synthesized Faujasite (FAU-1), (FAU-2) and (FAU-3).**

Material from Departure	**H_2O Deformation mode**	**Stretching Asymmetrical [a]**	**Stretching Symmetrical [b]**	**Structure D6r**
FAU-1	1634	993	685	566
FAU-2	1643	994	676	558
FAU-3	1634	991	679	565

[a] Al-O of the structure Si-O-Al

[b] Parallel rings of 6 members

3.2. Average results of the BET area of the synthesized products.

TABLE. 3. **Average surface area.**

Sample	**Average of Superficial area m^2/g**
FAU-1	177.44
FAU-2	195.13
FAU-3	118.52

TABLE. 3, shows the surface area of FAU-3, which is the smallest in comparison to the other samples, and FAU-2 has a larger surface area. For this reason, FAU-2 is the most appropriate for this type of study, with oil, in the case of TGA analysis.

3.3. Results of the mineralogical characterization by X-ray diffraction

TABLE. 4 shows the mineralogical characterization by XRD for the synthesized samples:

TABLE. 4. **Mineralogical characterization by XRD for the synthesized samples.**

Sample Synthesized	**Name**	**Formula**	**Sample Zeolite%**
FAU-1	Faujasite – Na	Na_{71} ((Si_{121} Al_{71}) O_{384})	2.6
	Amorphous material	------------------------	97.4
FAU-2	Faujasite – Na	Na_{71} ((Si_{192} Al_{192}) O_{384})	11.47
	Sodalite	($Na_4(Si_3Al_3)O_{12}Cl$)	88.52
FAU-3	Faujasite – Na	Na_{71} ((Si_{121} Al_{71}) O_{384})	2.6
	Spectrolyte	(Ca Na) (Si Al $)_4$ O_8	1.9
	Aluminum sodium silicate Hydrated	$Na_2.0_6$ Al_2 $Si_3.8$ $O_{11}.63$!8 H_2 O	1.3
	Amorphous material	------------------------	94.2

The Sodalite or regular octahedron cube is the basic unit of Faujasite, which is present in the FAU-2 synthesized sample with 88.52% and 11.47% Faujasite, whereas in FAU-1 and FAU-3 2, 6% faujasite without presence of Sodalite.

TABLE. 5. **Number of Tetrahedrons per unit cell (TO_4).**

Sample	**Atom**	**Number of tetrahedrons per unit cell (to_4)**	**Position**		
			x	y	z
FAU-1	Al	192	0.96	0.67	0.05
	Si	192	0.96	0.67	0.05
FAU-2	Al	71	-------	-------	-------
	Si	121	-------	-------	-------
FAU-3	Al	71	-------	-------	-------
	Si	121	-------	-------	-------

The results for FAU-2 give a Si/Al ratio of 1 corresponding to 192/192 atoms of each element. For FAU-1 and FAU-3 the results give a ratio of 1.70 corresponding to the Si/Al ratio of 121/71.

For the results obtained from FAU-2 contains less acidic centers, they are high in all three cases but even more active when the amount of aluminum atoms decreases or when the Si/Al ratio increases as in the case of FAU-1 and FAU-3, it should be noted that not all acidic centers possess equal activity and therefore not all are capable of catalyzing a given chemical reaction, but only those possessing sufficient strength to do so.

In the synthesized samples FAU-1, FAU-2 and FAU-3 the XRD analysis was performed, affirming the effect that the synthesized material is treated as faujasite because the number of tetrahedra per unit cell is 192 for each case characteristic of the zeolite. In FAU-1 and FAU-3, 2.6% was obtained and in FAU-2, 11.47% faujasite was obtained as shown in TABLE. 5. In the FAU-2 synthesized sample, the basic unit of Faujasite which is sodalite or cube octahedron regular with 88.52% indicating that the unit of the faujasita could not complete its structure that could be carried out by means of a modification of the hydrothermal treatment.

Due to the high amount of amorphous material observed in the obtained diffractogram and the present sodalite, it is necessary to study the variation of other synthesis parameters, for example, the composition as Si/Al ratio of the natural clinker, which has an important Influence on the acidity of the same, property characteristic of the zeolites.

3.4. Characterization of the BET area test using the GCMC simulation

The software Medea@2.15 was used in which the BET area was simulated using the Monte Carlo Granular Method (GCMC) (MEDEA-GIBBS) to obtain the specific area of the pore (s).

TABLE. 6. **FAU-2 Crystal data results.**

Settings of Cell		**Software MEDEA**	**Experimental Method***
(Å)	a	24,34	24,92
	b	24,34	24,92
	c	24,34	24,92
(°)	α	90	90
	β	90	90
	γ	90	90
* X-ray diffraction results			

TABLE. 7. **Comparison of Medea cell volume and synthesized samples.**

	Compound	**Formule**	**Volume, Å^3**
Faujasite Na56Y (Simulated)	Faujasite-Na56Y	$Na_{46}Si_{192}O_{384}$	14428,77
FAU-1	Faujasite-Na	$Na_{71}((Si_{121}A_{l71})O_{384})$	15523,97
FAU-2	Faujasite-Na	$Na_{71}((Si_{192}Al_{192})O_{384})$	15453,16
FAU-3	Faujasite-Na	$Na_{71}((Si_{121}A_{l71})O_{384})$	15523,97

The cell volume of the experimentally synthesized faujasite is different from the result obtained by simulation, due to the quantity of zeolitic material of the sample obtained.

TABLE. 8. **Comparison of surface areas simulation and BET equipment.**

Superficial Area m^2/g		
Sample	**Simulation Method N_2 BET a 77K, GCMC**	**Experimental Method BET N_2 a 77K**
Faujasite Na56Y (Simulated)	137.21	----
FAU-1	----	177.44
FAU-2	----	195.13
FAU-3	----	118.52

3.5. Thermogravimetric analysis (TGA)

For the catalytic cracking analyzes, a TGA 1 equipment was used, varying the faujasite/heavy crude ratio in the range of 0.05 to 0.005 at a temperature of 420°C. FAU-1 was used as an example. For the catalytic cracking tests, FAU-2 was used since as indicated above this presented the best results in the physical characterization.

FIG. 4, shows the thermogravimetric curves for each of the relationships. Each curve corresponds to the average of three replicate assays.

FIG 4. **Diagram of mass loss of heavy crude oil.**

FIG. 4 shows the thermogravimetric curves of heavy crude with and without zeolite. When comparing the results it is observed that as the amount of faujasite decreases, a higher rate of gas generation is obtained. The mass loss of the heavy crude was higher with a ratio of 0.01; this is a very satisfactory result taking into account that the purity of the faujasite used was of 11.475%.

4. Conclusions

- The results obtained for the characterization of the tests performed in the XRD and FT- IR, it was verified that the zeolite obtained is faujasite, since the crystallization time in the hydrothermal treatment is not necessary due to the greater percentage of amorphous material that was obtained in the experimentation.

- The value of tetrahedra obtained per unit cell (TO_4) of the synthesized zeolite is 192, indicating the validity of the zeolite which is of faujasite type, thus verifying this process of synthesis by alkaline fusion.

- By increasing the time interval for the hydrothermal treatment in order to obtain a greater crystallization of zeolite type faujasite, for the three materials 11.47% of natural clinker was obtained in crystal form while the others a value of 2.6%.

- The aluminum atom content of 192 for FAU-2, FAU-1 and FAU-3 is 71 atoms of aluminum according to the DFX method, determining FAU-2 to contain active acid centers.

- Comparing the BET surface area of the theoretical faujasite compared to the faujasite obtained experimentally by the Great Canonical Monte Carlo method, it was verified that they are not similar numerically because their chemical formula is different considering that it has amorphous material, giving validity to the method of simulation considered as characterization test.

- TABLES. 6-8, concludes that the experimental method of synthesis crystallized Faujasite type zeolite because the parameters of the software glass and those of the experimental method are similar numerically.

- Experimentally, according to FIG. 2, it was demonstrated that the faujasite possesses catalytic activity, obtaining a greater generation of cracked gases with a zeolite/crude ratio of 0.01%.

Acknowledgment

To the Oil Public Company in Ecuador. EP. PETROECUADOR. The results obtained from the DRU of FAU-1 and FAU-3 were performed in the Laboratory of Metrology and Materials Testing (LEMAT) and the FAU-2 results in the Proinstra Laboratory.

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