



41ª Reunión Ibérica de Adsorción

3^{er} Simposio Iberoamericano de Adsorción

5-7 septiembre/setembro/September 2018 · Gijón, Asturias (España)

ABSTRACTS BOOK



**41ª Reunión Ibérica de Adsorción - 3^{er} Simposio
Iberoamericano de Adsorción**

**41ª Reunião Ibérica de Adsorção - 3º Simpósio Ibero-
Americano de Adsorção**

41st Iberian Adsorption Meeting - 3rd Iberoamerican
Adsorption Symposium

Palacio de Congresos de Gijón, Sala Anfiteatro
Recinto Ferial Luis Adaro, Gijón
5-7 Septiembre/**Setembro**/September 2018

Organized by:



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VENUE

Conference. Gijón Convention Center. Av. Dr. Fleming, 481, Gijón

Adsorption School.

Tuesday. Casino de Asturias, Sala Acapulco, Fernández Vallín St., 5, 33205, Gijón

Wednesday-Friday. Gijón Convention Center. Av. Dr. Fleming, 481, Gijón

Iberoamerican Women Scientists Round Table (OPEN ACTIVITY). Antigua Escuela de Comercio, Francisco Tomás y Valiente St., 33201 Gijón

Opening Ceremony and Welcome Cocktail. Casino de Asturias, Sala Acapulco. Fernández Vallín St., 5, 33205, Gijón.

Adsorption at the pub (OPEN ACTIVITY). Savoy, Covadonga St, 5, 33202 Gijón

Gala Dinner. Bellavista Restaurant, Av. José García Bernardo, 256, 33203, Gijón



Separation of C₅/C₆ isomerase fractions in a mixed/layered bed of BETA/5A Zeolites

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Introduction

The combustion quality of gasoline is measured by the research octane number (RON). When RON is high, the combustion occurs like a smooth explosion instead of a detonation and the performances of the motor are improved. Cracking, alkylation, isomerization and other process can be used to increase the RON of gasoline to about 90. The light straight-run (LSR) naphtha fraction produced by fractional distillation is one of the feedstocks used to produce gasoline. Its major constituents include C₅ and C₆ normal paraffins which have relatively low RON compared to their branched isomers. Therefore, octane upgrading commonly uses isomerization to rearrange the structure of the linear paraffins into branched components. The product stream from an isomerization reactor consists of hexane isomers: 2,2-dimethylbutane (22DMB), 2,3-dimethylbutane (23DMB), 2-methylpentane (2MP), 3-methylpentane (3MP), *n*-hexane (nHEX), as well as pentane isomers: *iso*-pentane (iPEN) and *n*-pentane (nPEN).

Zeolite 5A is used to separate the linear isomers (nHEX and nPEN) from the branched isomers, returning them to the isomerization reactor for further processing, while the other isomers are retained as product. Denayer et al. [1] found that pentane and hexane isomers might be separated by chromatography according to their degree of branching using columns of zeolite beta, and some years before Huddersman and Klimczyk [2,3] indicated that zeolite beta in cation form (H, Ba) is an effective adsorbent for the separation of branched hexane isomers. Therefore, using both zeolites together should allow for a better separation of the high RON isomers (22DMB, 23DMB and iPEN) from the remaining isomers, specially the low RON isomers (nPEN and nHEX). Thus, four different adsorber bed configurations were studied: zeolite beta; a layered bed of zeolite 5A followed by zeolite beta; a layered bed first with zeolite beta followed by zeolite 5A; and, a mixed bed of both zeolites with the objective of analyzing the effect of each configuration on the adsorption and separation of alkane isomers.

Experimental

Zeolite beta in the H⁺ form was purchased from Süd-Chemie AG, Clariant, in form of pellets of 1/16 inches under the reference H-BEA 150. Zeolite 5A was purchased from Chemiewerk Bad Koestritz in binderless form. Helium is used as carrier gas as well as solvent for the alkane isomers mixture. 5679.9 mg of zeolite beta were used for single adsorber experiment; and, 4025.9 mg of zeolite beta together with 2131.4 mg of zeolite 5A were used in the layered as well as in the mixed bed experiments for a total mass of 6184.3 mg of adsorbent. An equimolar mixture of pentane and hexane isomers (22DMB, 23DMB, 2MP, 3MP, nHEX, iPEN, and nPEN) was used for all experiments. They were all carried out at 423 K and total isomers pressure equal to 0.50 bars. This pressure is reached by diluting a flow of isomers mixture of 81.01 μmol/min with a Helium flow of 1.84 ml/min which corresponds to double of the hydrocarbon molar flow, resulting in a total partial pressure of 0.50 bars for the isomer mixture.

Results and discussion

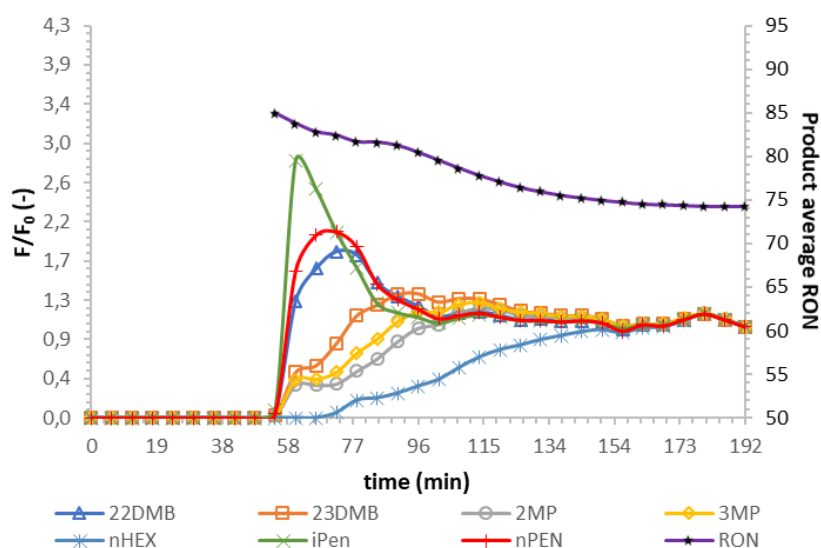


Figure 1. Breakthrough curve for an equimolar mixture of 22DMB, 23DMB, 2MP, 3MP, nHEX, iPEN, and nPEN at 423 K and total isomers pressure of 0.50 bars on a bed of zeolite beta.

Figure 1 shows the breakthrough curves for the experiment with zeolite beta. The adsorption hierarchy is nHEX >> 2MP > 3MP > 23DMB >> 22DMB > nPEN > iPEN. The purple curve is the average RON for the mixture (RON_{mix}) calculated based on the RON values of each isomer presented in Table 1 using the following expression:

$$RON_{mix} = \frac{\sum n_i \times RON_i}{\sum n_i}$$

Since nPEN leaves the column together with iPEN and 22DMB, this results in an average RON of 85 which then drops when 2MP and 3MP exit, even with 23DMB (the highest RON isomer) leaving

together with these isomers, this is not enough to compensate for all these low RON isomers. Then, the RON goes further down when nHEX starts to leave the adsorption column at around 70 minutes. Therefore, the maximum RON obtained is 85 which is the value when the breakthrough curves begin, showing that further work is necessary to improve the separation and consequently the RON obtained.

Table 1. Isomers' RON number [4].

Alkane isomers	RON
2,3-dimethylbutane (23DMB)	101.7
Isopentane (iPEN)	92.3
2,2-dimethylbutane (22DMB)	91.8
3-methylpentane (3MP)	74.5
2-methylpentane (2MP)	73.4
Normal Pentane (nPEN)	61.7
Normal Hexane (nHEX)	24.8

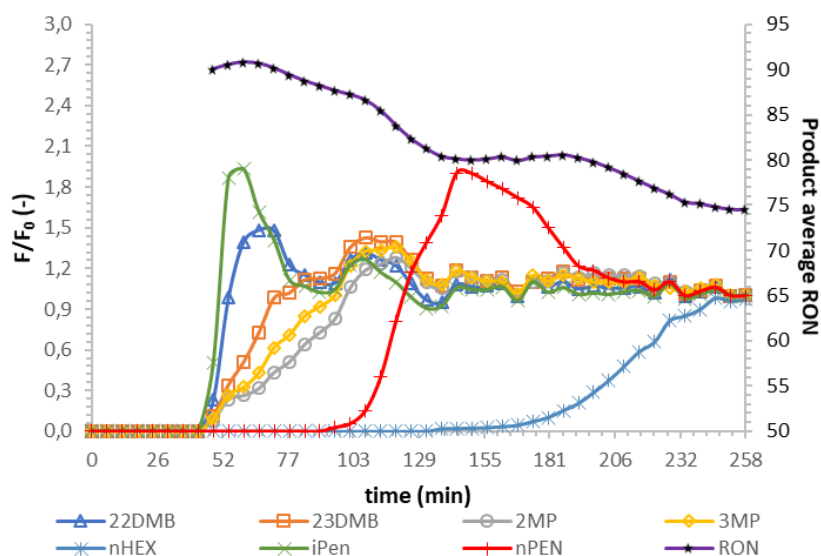


Figure 2. Breakthrough curve for an equimolar mixture of 22DMB, 23DMB, 2MP, 3MP, nHEX, iPEN, and nPEN at 423 K and total isomers pressure of 0.50 bars on a layered bed of zeolite 5A and zeolite beta.

Figure 2 presents the breakthrough curves of a layered bed of zeolite 5A and zeolite beta. The presence of zeolite 5A makes the linear isomers leave the column later than in the experience with zeolite beta, with nPEN and nHEX respectively exiting 50 and 60 minutes later than in the previous experiment. Thus, the adsorption hierarchy on the layered bed of zeolite 5A and zeolite beta is: nHEX >> nPEN >> 2MP > 3MP > 23DMB > 22DMB > iPEN. This is results in a high RON value

of 90 when iPEN and 22DMB exit the column, which then starts to drop when the 2MP and 3MP leave the adsorption column. The RON stabilizes due to the overshoot of the breakthrough curve of nPEN but it decreases again when nHEX finally exits the adsorption column and the concentration of nPEN normalizes.

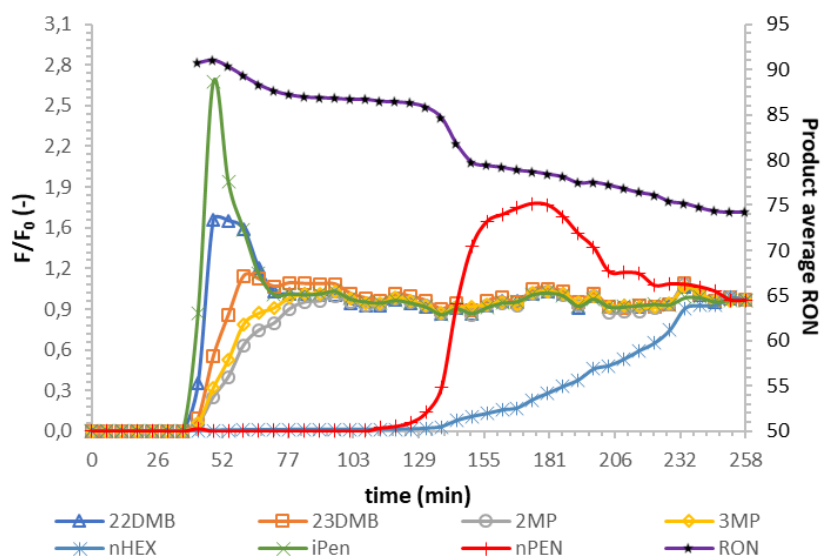


Figure 3. Breakthrough curve for an equimolar mixture of 22DMB, 23DMB, 2MP, 3MP, nHEX, iPEN, and nPEN at 423 K and total isomers pressure of 0.50 bars on a layered bed of zeolite beta and zeolite 5A.

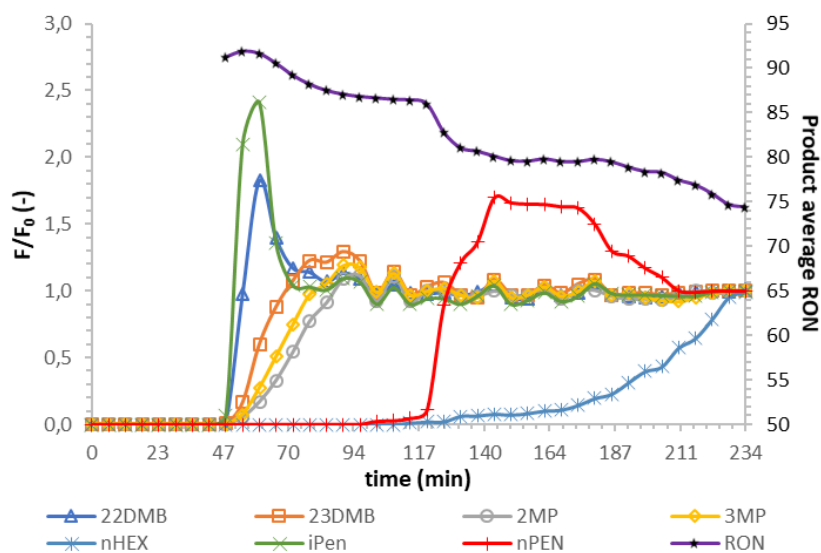


Figure 4. Breakthrough curve for an equimolar mixture of 22DMB, 23DMB, 2MP, 3MP, nHEX, iPEN, and nPEN at 423 K and total isomers pressure of 0.50 bars on a mixed bed of zeolite 5A and zeolite beta.

In Figure 3, the breakthrough curves of a layered bed of zeolite beta followed by a layer of zeolite 5A are shown. This configuration makes the nPEN exit the column later than in the other layered bed experiment, almost at the same time as nHEX. Regarding the remaining isomers, there is no

significant change in their adsorption, resulting in an adsorption hierarchy of: nHEX > nPEN >>> 2MP > 3MP > 23DMB > 22DMB > iPEN. The maximum RON obtained for this configuration is 91, which is slightly higher than the one obtained in the layered configuration with the opposite order of layers (5A then Beta) due to 23DMB having a higher overshoot than in the previous experiment.

Figure 4 presents the breakthrough on a mixed bed with zeolite 5A and zeolite beta. Once again, the presence of zeolite 5A increases the adsorption of the linear isomers, making them leave the column after all the other isomers, and as in the layered bed of zeolite beta and zeolite 5A. nPEN exits the column close to nHEX. The adsorption hierarchy is the same as in the previous test: nHEX > nPEN >>> 2MP > 3MP > 23DMB > 22DMB > iPEN. The maximum RON obtained is 91 which is the same as the previous experiment.

Conclusions

Using zeolite 5A together with zeolite beta improves the separation of alkane isomers, increasing the RON of the mixture by making the linear isomers, which have the lowest RON, exit the adsorption column much later than in the experiment with only zeolite beta. Concerning the different absorber bed configurations studied, the layered bed of zeolite beta followed by zeolite 5A and the mixed bed show the best results with a maximum RON of 91 and significantly increasing the separation of branched isomers from the linear isomers.

Acknowledgements.

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