

XVIII ENCONTRO LUSO-GALEGO DE QUÍMICA

09:00 - 09:50	PL 3 – Jorge Calado , Departamento de Engenharia Química, Instituto Superior Técnico <i>A História da Energia</i>			
Chairperson Salas	Comunicações Oraís	Auditório 1	Auditório 2	Auditório Geociências
09:50 - 10:40		Química Fundamental	Química e Energia	Química Ambiental
	09:50 - 10:05	F-7	ENER-4	AMB-4
	10:05 - 10:20	F-8	ENER-5	AMB-5
	10:20 - 10:35	F-9	ENER-6	AMB-6
	10:35 - 10:40	<i>Discussão</i>	<i>Discussão</i>	<i>Discussão</i>
10:40 - 11:20	Café, discussão de painéis e sessão de autógrafos (Prof. Jorge Calado)			
Chairperson Salas	Comunicações Oraís	Auditório 1	Auditório 2	Auditório Geociências
11:20 - 13:00		Química Fundamental	Química Alimentar	Química Industrial
	11:20 - 11:35	F-10	AMA-4	IND-7
	11:35 - 11:50	F-11	AMA-5	IND-8
	11:50 - 12:05	F-12	AMA-6	IND-9
	12:05 - 12:10	<i>Discussão</i>	<i>Discussão</i>	<i>Discussão</i>
	12:10 - 12:25	F-13	AMA-7	IND-10
	12:25 - 12:40	F-14	AMA-8	IND-11
	12:40 - 12:55	F-15	AMA-9	IND-12
	12:55 - 13:00	<i>Discussão</i>	<i>Discussão</i>	<i>Discussão</i>
13:00 - 15:00	Almoço			
Chairperson Salas	Comunicações Oraís	Auditório 1	Auditório 2	Auditório Geociências
15:00 - 16:40		Química Fundamental	Educação e Ensino	Química Ambiental
	15:00 - 15:15	F-16	EDU-1	AMB-7
	15:15 - 15:30	F-17	EDU-2	AMB-8
	15:30 - 15:45	F-18	EDU-3	AMB-9
	15:45 - 15:50	<i>Discussão</i>	<i>Discussão</i>	<i>Discussão</i>
	15:50 - 16:05	F-19	EDU-4	AMB-10
	16:05 - 16:20	F-20	EDU-5	AMB-11
	16:20 - 16:35	F-21	EDU-6	AMB-12
	16:35 - 16:40	<i>Discussão</i>	<i>Discussão</i>	<i>Discussão</i>
16:40 - 17:30	Café e discussão de painéis			
17:30 - 18:20	Comunicações Oraís	Química Fundamental	Bioquímica	Química Ambiental
	17:30 - 17:45	F-22	BB-1	AMB-13

Single and multicomponent sorption of hexane isomers on MOF ZIF-8

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The chemical nature of Metal-Organic Frameworks (MOFs) based in a hybrid skeleton that combines inorganic building bricks (or Secondary Building Units – SBU) together with organic linkers present a system with several degrees of freedom that can be explored to solve specific separation problems. If the organic linker is an anionic N donor of the imidazolate-type we can obtain the so-called ZIF frameworks. Twelve frameworks were synthesized by combining a metal salt with imidazole type linkers [1]. One of such frameworks, ZIF-8, possesses a superior chemical stability with a surface area around 1810 m²/g.

The main goal of this research focuses on the development of an adsorptive process to separate hexane isomers (kinetic diameter very similar) in order to improve the quality of gasoline measured by the octane number (RON). In this investigation, studies of sorption equilibrium of hexane isomers: n-hexane (RON 25), 3-methylpentane (RON 75), 2,3-dimethylbutane (RON 103) and 2,2-dimethylbutane (RON 94) were performed on ZIF-8. The MOF ZIF-8 was synthesized and fully characterized by XRD, TGA, IR and surface area at the Institute Lavoisier Versailles.

To achieve the objectives, we have performed a set of screening studies for quaternary mixtures of hexane isomers (figure 1), measuring at the same time single and multicomponent sorption isotherms. The temperature range 323-423 K and partial pressures up to 30 kPa have been explored. Figures 1 shows a typical multicomponent equimolar breakthrough experiment of hexane isomers on ZIF-8. For all experiments, the sorption hierarchy in ZIF-8 is: nHEX>>>3MP>23DMB>22DMB. The results obtained show that MOF ZIF-8 can be effective for separating nHEX from the branched isomers with working capacities that can reach 35 wt%, which can be considered a huge value when compared to sorption of paraffins in zeolites. Further studies are now being developed to increase the degree of separation.

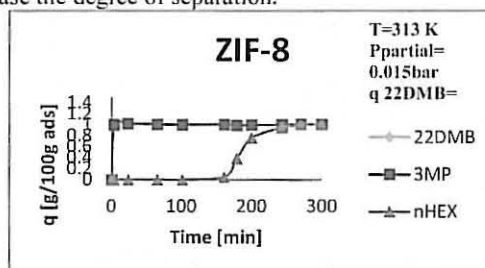


Figure 1 – Multicomponent breakthrough experiment of hexane isomers on ZIF-8.

References:

- [1] Omar Yaghi et al., Exceptional chemical and thermal stability of zeolitic imidazolate frameworks. The National Academy of Sciences of the USA, July 5, 2006, Vols. vol. 103, no. 27, 10186–10191.