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Separation of branched hexane isomers on zeolite BETA

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In a world aware of the end of cheap oil, it is time to research for solutions that can optimize even more the performances of the carburant, increasing the efficiency of the vehicle motors. In the case of gasoline, the combustion quality, measured by the research octane number (RON), can be improved removing low octane paraffins from the gasoline. For instance, n-hexane (nHEX) and 3-methylpentane (3MP) exhibits a low RON, whereas 2,2-dimethybutane (22DMB) and 2,3-dimethybutane (23DMB) are high RON molecules. These four isomers are the major constituents of the output of Total Isomerisation Processes (TIP) and their molecular kinetic diameter is similar, which makes the separation difficult. In order to improve the TIP, this study focuses on the development of an adsorptive process to separate monobranched from dibranched C_6 isomers producing a high octane cleaner burning gasoline.

An experimental study of single and binary fixed bed adsorption of C_6 isomers was performed covering a temperature range between 423 K and 523 K and partial pressures up to 0.3 bar. The effect of partial pressure and temperature in the shape of breakthrough curves was addressed. From these data single and binary adsorption equilibrium isotherm were collected. Based on the analysis of sorption events at the molecular level, two different models were used to interpret with a good accuracy the equilibrium data: dual-site Langmuir (DSL) for nHEX and 3MP and multi-site Langmuir (MSL) for 23DMB and 22DMB. At the partial pressures studied it was found that the affinity of the isomers to the zeolite is: nHEX >>> 3MP > 23DMB >> 22DMB. Figure 2 shows a binary breakthrough curve of a mixture of a monobranched (3MP) and a dibranched (22DMB) molecule. It is clear from this figure that BEA structure demonstrates a significant selectivity between branched C_6 isomers, especially at low coverage, giving a good perspective regarding future works.

The IAST using the DSL model to describe the pure component equilibrium of nHEX and 3MP and the MSL model for the dibranched isomers 22DMB and 23DMB give a good prediction of the mixture adsorption data. Thereafter, a dynamic adsorption model was developed and tested predicting with a good accuracy the behaviour of the fixed bed experiments.

The results arising from this study are opening a window to solve the separation problem between monobranched and dibranched C_6 isomers. These data are now being used in the development of a cyclic process by an appropriate technology.

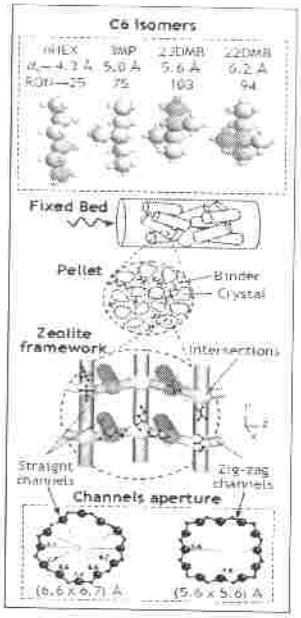

Figure 1. Illustration of a fixed bed adsorption process showing the various levels of porosimetry. The figure also includes: a 3D view of C_6 isomers and kinetic diameters; a perspective view of the zeolite BETA framework with the 12-ring pore apertures.

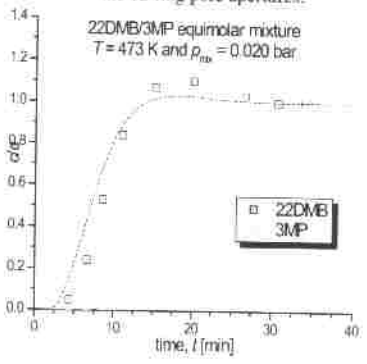

Figure 2. Binary breakthrough curve for a mixture of 22DMB/3MP in zeolite BETA. Points are experimental data and lines are dynamic model simulation.