Spider Application Note

Development of a low temperature paraffin isomerisation catalyst

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Traditionally platinum on chlorinated alumina has been the catalyst used for low temperature (140°C) isomerisation of n-C_5 and n-C_6 paraffins (light straight run gasoline). Pt on zeolites (mordenite) is the catalyst used of high temperature LSR isomerisation processes. The Pt/zeolite is a more robust catalyst towards water and sulphur deactivation, but the octane number of the gasoline produced with mordenite is lower than that obtained with the chlorinated alumina.

Platinum on sulphated zirconia and tungsten oxide on zirconia are active and selective catalysts for carrying out the isomerisation of n-C5 and n-C6 paraffins at temperatures lower than zeolites but higher than Pt on chlorinated alumina. However, these catalysts are highly sensitive to water and sulphur in the feed.

A search for a new, more water and sulphur resistant catalyst for low temperature isomerisation of light paraffins was conducted using genetic algorithm optimisers. Each catalytic material is represented by a set of parameters, and through a genetic evolution the fittest materials have a tendency to yield good quality offspring.

Isomerisation of *n*-pentane was chosen as a model isomerisation reaction of light alkanes. Fundamental knowledge was applied to design the catalytic parameters and rules for combination of the search algorithm, and with these, highly active and selective catalysts obtained.

High throughput testing was carried out in the Spider16 reactor system, which is able to work at up to 70 bar and 600°C. Each reactor is independently fed using one liquid and one gas mass flow controller, making it possible to operate in the contact time range of 0.1-2h for an H_2/*n*-pentane ration of 2.93 mol/mol and 500mg of catalyst. Temperature and pressure are also measured in each catalyst bed.

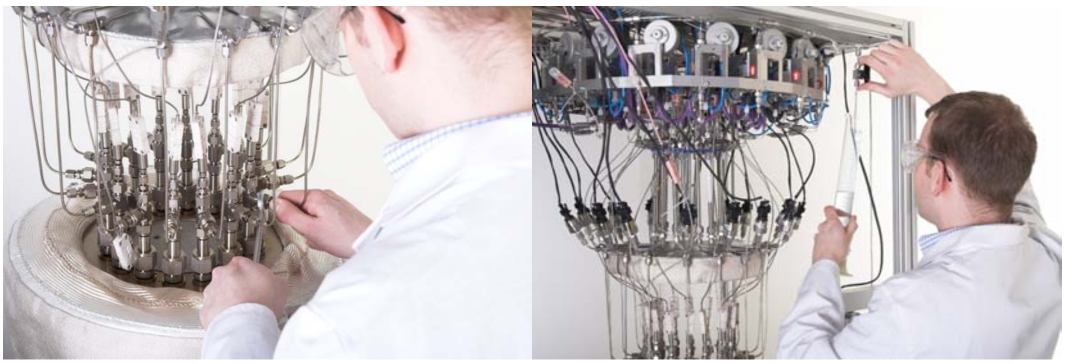

Figure 1 Spider System

The system is designed so that calcination and reduction can be performed in the Spider system prior to the activity test. Calcination was performed at 600°C in air for eight hours and reduction in hydrogen at 250°C for two hours.

Catalytic testing was carried out at 30 bar, temperature between 200 and 240°C and contact time of 0.44h, H_2/hydrocarbon ratio 2.93 mol/mol. The amount of catalyst in each reactor used was 500mg with a particle size in the 400-600µm range, where there are no internal diffusion limitations. Product distribution was analysed using a fast GC, the system was optimised to reduce the total cycle time required for each analysis procedure.

The number of catalysts in each generation was fixed at 24, and after each activity test the optimisation algorithm designed the next set of catalysts, taking into account the compositions and catalytic performances of the prior generation. For n-pentane isomerisation the performance is practically equal to the n-pentane conversion due to the low cracking activity of the catalysts.

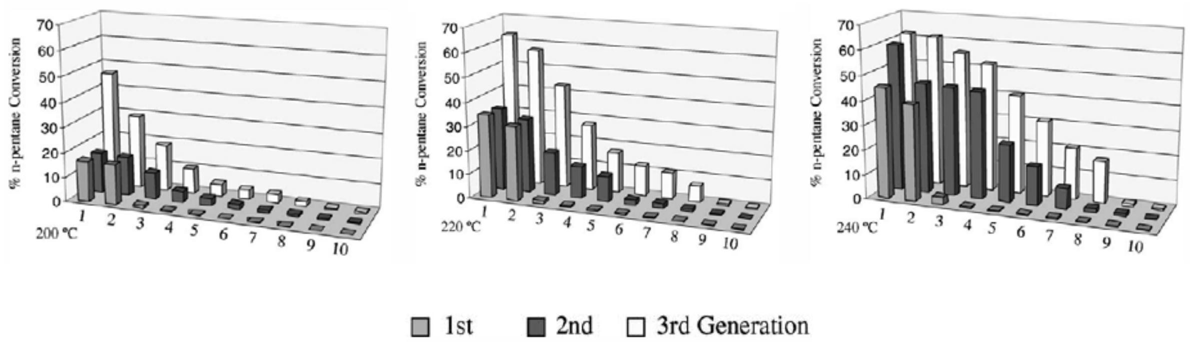

Figure 2 Isomerisation performance of 10 best ranked materials in 3 generations

Three evolving cycles were run, figure 2 shows the catalytic performance of the 10 most active catalysts for the 3 generations at three different reaction temperatures. An important improvement in the activity can be observed during the evolution.

Original Article

Development of a low temperature light paraffin isomerization catalysts with improved resistance to water and sulphur by combinatiorial methods

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