Question 45: What tools are you using to predict the yields of Xylene, Benzene, Toluene and other aromatics in a catalytic reformer? What methods do you use and how often do you test the feedstock for these variables? Other than feedstock quality, what factors are you accounting for in the individual yields (unit pressure, RON, etc)? Do you have any rules of thumb for conversion of certain species of aromatics?

Olivier Le-Coz (Axens)

Dedicated simulators are run for prediction, either using correlations or kinetic models. To be able to perform accurate predictions, feed analyses shall be performed every time the feedstock quality is changed: the most important one is detailed hydrocarbon analysis by gas chromatography (for instance Carburane).

The main parameters that impact yields and aromatic content in the reformate are of course pressure, H2/HC ratio, residence time (modeled through WHSV or GHSV), catalyst temperature and catalyst selectivity factors. Moreover, the chloride content is also a parameter to take into account for the evaluation of the aromatic's distribution.

Erik Myers (Valero)

At our refinery where this is applicable, we utilize a combination of our Profimatics / corporate modeling along with the licensor developed spreadsheet model. We utilize weekly mass balanced data along with gas chromatograph product results and feed and reformate PONA analyses. Yields can be normalized for pressure and severity. Goals are to minimize pressure, minimize chloride on catalyst and minimize octane (severity) for increased C5+ yield. Conversion rules of thumb are: Naphthene's are fast, paraffins are slow. C5 rings lead to large liquid loss, C6 rings are preferred.

Valero also recommends use of a PONA grid for better modeling of reforming feed stocks where the C5 and C6 rings are identified for each carbon number. For example, ethyl-cyclopentane and methyl-cyclohexane are both C7 naphthenes but the conversion of methyl-cyclohexane to toluene is much better with the C6 naphthene ring. In fact, the assumption of the distribution of C5 and C6 rings is the fundamental modeling error in reforming. Coker naphthas and synthetic crudes oils are enriched in the C5 rings relative to the C6 rings.

Brad Palmer (ConocoPhillips)

Switching to aromatic production mode is determined by the LP model according to market demand and

economics. Operation of the naphtha hydrotreater, Reformer and Aromatic Extraction unit is set by the mode of operation (gasoline mode or aromatics mode) without use of additional modeling or predictive tools.

High quality feed (high N+2A) and higher Reformer severity increases aromatic production; therefore, when an aromatics mode is desired, the highest quality feeds are routed to the Reformer, the severity is increased, and the catalyst circulation is increased to keep up with increased coke production.

Aromatic Extraction unit operation is also changed to handle the increased aromatic concentration: solvent to feed ratio is increased, tertiary solvent is started and raffinate recycle to feed is started to maintain an optimum feed concentration.

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