

## PERP Program – Optimizing Aromatics Production

### New Report Alert

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Nexant's *ChemSystems* Process Evaluation/Research Planning program has published a new report, ***Optimizing Aromatics Production (05/06S6)***. To view the table of contents or order this report, please click on the link: <http://www.chemsystems.com/reports/index.cfm?catID=2>

#### INTRODUCTION

Most new aromatics complexes are designed to maximize the yield of benzene and *para*-xylene. Benzene is a versatile petrochemical building block used in many different products based on its derivation including ethylbenzene/styrene, cumene/phenol and cyclohexane/caprolactam. *para*-Xylene is used almost exclusively for the production of polyester fibers, resins and films formed via terephthalic acid (PTA) or dimethyl terephthalate (DMT) intermediates. An aromatics complex may be configured in many different ways depending on the desired products, available feedstock and investment capital available and there are a variety of technologies for license to accomplish this goal.

In the past optimization for aromatics complexes consisted mainly of economy of scale. In the past 10 years technical improvement have allowed the single train size for *para*-xylene recovery to be expanded from a range of 400-500 kta to 600-700 kta. Another area in which there has been improvement is in the efficiency of converting the naphtha feed to *para*-xylene. This has primarily been done through improvements in various catalysts, such as Axens' AR 501 and UOP's R-264 reforming catalyst. Finally improvements in processing heavy aromatics for conversion to xylenes have enhanced the overall efficiency of the aromatics complex.

The two patented processes reviewed in this report, approach optimization of an aromatics facility from two different perspectives. CPCC uses existing catalysts and technologies to maximize the production of *para*-xylene without consideration for the other aromatics (e.g., benzene). On the other hand, UOP uses its proprietary technologies to reduce the cost of investment, simplify the flow scheme, and, thus, the cost of production of *para*-xylene, while still producing benzene as a by-product. The optimizations are not comparable to each other, but are evaluated based on discrete base cases developed specifically for this evaluation.

## CPCC PATENT

China Petroleum and Chemical Corporation (CPCC) has patented a process flow scheme for producing *para*-xylene that they claim can increase the output of *para*-xylene by 36 percent over a conventional process (re: U.S. patent 6,867,339). The units included in this configuration consist of an adsorptive/isomerization unit, a selective toluene disproportionation unit (STDP), fractionation columns (deheptanizer, xylenes column, benzene column, toluene column, heavies column) and an aromatics alkyl transfer unit (SATP). This invention feeds benzene, as well as C<sub>9</sub> aromatics, to the alkyl transfer unit to produce toluene and mixed xylenes. Thus, all the benzene, toluene and C<sub>9</sub> aromatics are recycled to extinction. The only products produced are *para*-xylene, non-aromatics and C<sub>10+</sub> aromatics. A conventional configuration will normally recover benzene as well and have a yield of 50 to 60 percent *para*-xylene. The CPCC process will recover yields of over 80 percent *para*-xylene.

The conventional process for producing *para*-xylene is to separate *para*-xylene contained in the xylene stream (ethylbenzene, *meta*-xylene, *ortho*-xylene and *para*-xylene in an equilibrium mixture produced via catalytic reforming of naphtha) by multi-stage cryogenic crystallization separation or molecular sieve simulation moving bed separation (i.e., adsorptive separation). An isomerization process is generally used to isomerize the remaining isomers to an equilibrium mixture which is recycled to extinction. An effective route to increase the output of *para*-xylene is to disproportionate toluene (TDP) and transalkylate C<sub>9</sub> aromatics. Selective toluene disproportionation (STDP) produces a higher purity stream of *para*-xylene (i.e., greater than 80 percent) as opposed to the conventional TDP which produces an equilibrium mixture of xylenes (about 20 percent *para*-xylene). Various flow schemes and the chemistry are described in this report.

The CPCC patent has rearranged the conventional flow scheme to maximize *para*-xylene production. One of the major differences in the CPCC invention is that the concept of the alkyl transfer reaction in the SATP unit differs from that of the traditional alkyl transfer reaction. The traditional feed is toluene and C<sub>9</sub> aromatics to produce mixed xylenes via transalkylation and benzene and mixed xylenes via disproportionation. The CPCC invention uses benzene and C<sub>9</sub> and higher aromatics as the feedstock to produce toluene and C<sub>8</sub>'s and in doing so minimizes or eliminates the production of benzene from the plant.

We estimate the capital investment for the CPCC route to *para*-xylene is higher than the conventional configuration by about \$40 million. This is due mainly to the additional STPD unit which makes up 90 percent of the additional cost. The ISBL investment by unit is detailed in the report.

The costs of production for *para*-xylene via the CPCC patent configuration and a conventional adsorption/isomerization/TPD configuration have been developed for a plant capacity based on a fixed amount of reformate feed (710 kta). For the conventional route this will produce 429 kta of *para*-xylene and about 160 kta of benzene. The CPCC route produces 600 kta of *para*-xylene only. The latter is equivalent to a world scale *para*-xylene complex.

The results show that for the first quarter of 2006 the conventional configuration results in a lower cash cost. The CPCC has lower by-product credits because no benzene is produced and higher utility costs due to the additional processing unit (STDP), but has lower fixed costs due to economy of scale of the adsorption and isomerization units. The CPCC configuration produces more *para*-xylene (600 vs. 429 kta) and no benzene and minor amounts of heavy aromatics. Although the cost of production and capital are higher for the CPCC configuration, the production of *para*-xylene and the yield are higher.

## UOP PATENT

UOP has patented an aromatics complex flow scheme that they claim significantly reduces the investment (re: U.S. patent 6,740,788). It requires that the reformer be operated at a very high severity (equivalent to producing about 104 to 106 RONC gasoline reformate) in order to maximize the production of aromatics. The invention eliminates the need for a reformate splitter, heavy aromatics column, benzene column and clay treaters after the reformate splitter and extractive distillation (i.e., Sulfolane) unit.

The high severity reformer operation extinguishes virtually all non-aromatic impurities in the C<sub>8</sub>+ fraction of reformate, and eliminates the need for extraction of the C<sub>8</sub> and C<sub>9</sub> aromatics. The transalkylation unit is designed to handle both C<sub>10</sub> aromatics and unextracted toluene. This allows the reformate splitter to be eliminated. No longer requiring a rigorous split between the C<sub>9</sub> and C<sub>10</sub> aromatics (i.e., feed to the transalkylation unit) allows the heavy aromatics column to be eliminated. The addition of the Olefin Reduction Process (ORP) eliminates the need for the clay treaters. The ORP unit selectively hydrogenates the olefins in the reformate to their corresponding alkane or cycloalkane. UOP claims that the new flow scheme will save 8 to 9 percent on the ISBL investment. The key to the UOP flow scheme is the ability of the Tatoray Unit (transalkylation process) to handle both C<sub>10</sub> aromatics and unextracted toluene. No longer needing to extract toluene allows the reformate splitter column to be eliminated and a smaller extraction unit for the recovery of benzene only. No longer requiring a rigorous split between the C<sub>9</sub> and C<sub>10</sub> aromatics allows a heavy aromatics column to be eliminated. To accomplish the latter the transalkylation catalyst is stabilized

through the introduction of a metal function. Finally the clay treaters are eliminated in favor of selective olefin saturation (i.e., UOP's proprietary Olefin Reduction Process, OPR).

The capital investment for the conventional route and the patented UOP route to *para*-xylene and benzene is detailed in the report for a world scale plant (i.e., 600 kta) of *para*-xylene. This investment has an accuracy of plus or minus 30 percent. The patented route has eliminated the reformat splitter and clay treaters, added the olefins reduction unit (OPR), expanded the Tatoray stripper (to include a stabilization section for recovery of benzene), and expanded the xylenes column to recover C<sub>9</sub>/C<sub>10</sub> aromatics as a side stream.

The cost of production has been estimated for both the conventional and newly patented UOP route to aromatics. While, the patented UOP process shows a small improvement in the cost of production, this approach is very attractive in terms of the savings in capital investment.

## MARKET ANALYSIS

Regional market forecasts out to 2010 for benzene and *para*-xylene are provided in the report.

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