

## **PART 3 – AROMA CHEMICALS from PETROCHEMICAL FEEDSTOCKS**

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### **6 FEEDSTOCK ANALYSIS**

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There are only two commercial types of mixed m/p-cresol feedstocks available. These are MP 90% purity and MP 99% purity. Merisol ceased manufacture of MP96 about three years ago, and would only consider producing this product on a campaign basis. There are no other commercial sources of MP96.

#### **6.1 MP 90% purity**

The purity ranges between 85 – 90 % depending on the supplier. The impurity is xylenols, these products are therefore often referred to as MPX, mixed cresol and xylene mixtures. As this product is a naturally derived mixed cresol, there are only two producers of this product internationally, Merisol and Bayer in Germany. The long-term price has been indicated to be in the order of \$ 1,400/ton. Merisol's product is called MP45 and is a unique product falling into this category.

The use of MPX has a minimal affect on the economics. Although it is a cheaper feedstock than either MP96 or MP99, the effective price of the pure mixed cresols is slightly higher. At the indicative long-term price for MP90% purity of \$ 1,400/t, the effective cost of the pure cresols lies between \$ 1,560 - 1,650/t. This is in the range at which the benchmark analysis has been done in the previous milestone reports. Although MPX has been evaluated on a pilot scale, sufficient work has not been carried out to demonstrate fully the process impact of the xylenols. The initial results have indicated lower yields of pHB compared to the use of MP99.

#### **6.2 MP 99% purity**

There are 3 major producers of this product worldwide, including Merisol. The long-term price is approximately \$ 2,000/ton. The percentage of m- and p- cresol in the mixed stream are however different for each product. The producers of MP99 are Merisol (50% m-cresol: 50% p-cresol content), Bayer (70%: 30%), Mitsui (60%: 40%), and the Merisol (50%)/Sumitomo (50%) joint venture Sumika-Merichem (60%: 40%). Merisol and Sumitomo market the Sumika-Merichem product independently.

Merisol therefore has two sources of MP99. It produces MP 99 (50% m-cresol: 50% p-cresol) at a facility in the USA using natural feedstocks from Sasol in South Africa, and also obtains product from the Sumika-Merichem joint venture (60%: 40%). Bayer is not a merchant supplier of MP99. It is believed that its cash cost of production for MP 99 is too high to allow it to compete.

The price of MP99 is determined by the market for wire enamel solvents in the Far East and by the market for flame-retardants in the USA. In contrast, the price of p-cresol is

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determined by the market for Butylated Hydroxy Toluene. Since all of these markets are completely unrelated, the price of p-cresol is determined independently from that of MP99. Since 85% of world p-cresol production is derived synthetically from toluene and Merisol produces only 15% from the separation of naturally derived mixed cresols, Merisol is the price follower and not the price setter for p-cresol. However, due to its very large market share in mixed cresols and MP 99, Merisol is the price setter for both MPX and MP99.

### **6.3 Feedstock Options**

From a technology perspective the ideal feedstock would be a MP99 feedstock with a cresol composition of 50% m-cresol and 50% p-cresol. The only producer that can directly supply this composition would be Merisol from the feedstock arising from Sasol. Because of the delicate balance between MP99, MP90, MPX, m-cresol and p-cresol globally, Merisol ensures that this balance is carefully managed through optimum utilisation of their combined multiple capacity worldwide. Merisol uses linear programming to determine logistics, timing and storage to determine the cost and revenue impact of different placement of these products. Thus, although in principal there should be no problem to obtain a supply of this preferred feedstock, in reality what will be made available would depend on what is perceived to be in their best to maintain product balances and plant loadings.

Owing to the robustness of the pHB selective oxidation technology, lower quality feedstocks such as the MPX's can be used. An advantage of having a feedstock supplied by Merisol ex Sasol would be that this would link the upstream commodity industry with downstream fine chemical industry in South Africa.

The MP90 (an MPX) produced by Bayer is not traded as a commercial product. All of the MP90 is consumed internally.

The use of a MP 99 feedstock with a higher m- to p- cresol ratio that could be supplied by any of the other three producers, Mitsui, Sumitomo or Sumika-Merichem, would have an impact on the techno-economics of the project in one of two ways:

- The high m:p ratio of 60:40 affects either the yield of m-cresol i.e. lower, if a 100% conversion of p-cresol to pHB has to be achieved (m-cresol degradation due to more severe oxidation conditions required), or the purity of m-cresol, if lower than 100% conversion of p-cresol to pHB is accepted (unreacted p-cresol contaminates the m-cresol by-product because of the difficulty associated with physical separation of the two molecular forms of cresol ).
- If the m:p ratio is brought back to 50:50, by topping up with either commercially more expensive (Western/Japanese suppliers) or cheaper

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(Chinese suppliers) p-cresol, the overall feedstock becomes either more expensive or less expensive as the case may be.

As most of the Far Eastern produced MP99 are primarily sold into the wire enamel solvent markets, this product should be available at wire enamel solvent prices of between \$1,150 – 1,300/ton.

### **6.4 Conclusion**

There is therefore only a small pool of mixed cresol suppliers internationally, from which a suitable feedstock for the petrochemical aroma value chain can be sourced. The CSIR pHB-pAA technology has been demonstrated using the more expensive feedstock, MP99 in a 50:50 ratio, and has been positively evaluated on MP96. The benchmarking exercise, although performed on MP 96 as feedstock, is independent of the feedstock as the analysis determines the effective cost of the pure cresols (50:50) at which the technology is competitive.